COMBUSTION DIAGNOSTICS AND OPTICAL TECHNIQUES

Editor in Chief
P.K. Buah-Bassuah
COMBUSTION DIAGNOSTICS AND OPTICAL TECHNIQUES
ICS - UNIDO AND
UNIVERSITY OF CAPE COAST
LASER AND FIBRE OPTICS CENTRE
DEPARTMENT OF PHYSICS

PROCEEDINGS OF
WORKSHOP ON COMBUSTION DIAGNOSTICS AND
OPTICAL TECHNIQUES

HELD AT

THE UNIVERSITY OF CAPE COAST
CAPE COAST
5 - 10 JULY, 1999
Group Photograph

Group Photograph of invited Dignitaries, lecturers and participants at the Opening Ceremony of the workshop on Combustion Diagnostics and Optical techniques
Front row (from Left to Right)

Prof. A. Ayensu
INNS, CSIR, Accra, Ghana.

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Code 11113, Sudan.

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Sudan University of Science, Khartoum Post

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Dean, School of Engineering, KNUST, Kumasi,
Ghana.

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Min. of Environment, Science & Tech. Accra,
Ghana.

Hon. Mr. W.S. Parker
Ghana.

Chief Executive, Tema Oil Refinery Ltd. Tema,
Ghana.

Hon. Lt. Col. C.K. Agbenaza (rtd)
Central Regional Minister, Cape Coast, Ghana.

Pro. S.K. Adjepong
Vice-Chancellor, Univ. of Cape Coast, Cape
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Ms. Florence Agyei
CSIR, Accra.

Dr. P.K. Buah-Bassuah
Co-ordinator, Laser and Fibre Optics Centre
Univ. of Cape Coast, Cape Coast.

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ICS - UNIDO
AND
UNIVERSITY OF CAPE COAST

PROCEEDINGS OF
WORKSHOP ON COMBUSTION DIAGNOSTICS
AND OPTICAL TECHNIQUES

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Prof. G. Denardo
Prof. A. Ayensu

Editor-in-Chief

Dr. P.K. Buah-Bassuah

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Prof. F.O Akuffo
Dr. Abeiku Brew-Hammond
Mr. S. Akoto Bamford
Dr. A. Owusu
Dr. S.Y. Mensah
## National Organising Committee

<table>
<thead>
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<td>Mr. W.S. Parker</td>
<td>Tema Oil Refinery Ltd., Tema</td>
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<td>National Nuclear Research Institute</td>
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<td>Public Relations Dept. Ghana National Petroleum Corp. Tema</td>
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<tr>
<td>Prof. A. Ayensu</td>
<td>INSS, Centre for Scientific and Industrial Research, Accra.</td>
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<td>Dean, School of Engineering Kwame Nkrumah Univ. of Science Tech. Kumasi</td>
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<td>Department of Physics Ghana Atomic Energy Commission, GAEC Kwabenya.</td>
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<tr>
<td>Dr. P.K. Buah-Bassuah</td>
<td>Laser and Fibre Optics Centre University of Cape Coast</td>
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<td>Cape Coast.</td>
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**COURSE DIRECTORS**

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<tr>
<td>Prof. F.O. Akuffo</td>
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<td>Dr. P.K. Buah-Bassuah</td>
<td>Laser and Fibre Optics Centre, Univ. of Cape Coast, Cape Coast.</td>
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  Chief Executive, Tema Oil Refinery Ltd.

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  Dr. Milčko Danailov
  ICS-ICTP Laboratory for Lasers and Optical Fibres
  Synchrotron Radiation Facility
  Trieste, Italy

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  Central Regional Minister

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  Minister of Environment Science and Technology

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  Minister of Mines and Energy

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  Mr. W.S. Parker
  Chief Executive, Tema Oil Refinery Ltd.
CLOSING CEREMONY ADDRESS

CHAIRMAN’S OPENING REMARKS
Prof. Kobina Yankson
Dean, Faculty of Science, University of Cape Coast,
Cape Coast, Ghana.

SHORT ADDRESS
Dr. P.K. Buah-Bassuah
Local Organizer/Coordinator of LAFOC, University of Cape Coast,
Cape Coast, Ghana

GUEST SPEAKER’S ADDRESS
Mr. Tsatsu Tsikata
Chief Executive,
Ghana National Petroleum Corporation, Tema, Ghana.

CHAIRMAN’S CLOSING REMARKS
Prof. Kobina Yankson
Dean, Faculty of Science, University of Cape Coast,
Cape Coast, Ghana.

SCIENTIFIC SESSIONS AND PRESENTATIONS

COMBUSTION SYSTEMS AND MODELLING

Invited Lecture
Combustion Process, What is it?
KNUST, Kumasi, Ghana

Combustion Modelling
KNUST, Kumasi, Ghana

Introduction to Turbulent Combustion Modelling
D. Veynante, Director du Laboratoire EM2C
Laboratoire d’Energetique Moleculair et Macroscopic, France.
Improvement of the Modelling of Industrial Furnaces And Processes following Experimental Observations
J.P. Martin, Paris, France

MONITORING PROCESSES

Invited Lecture
Monitoring air pollutants in combustion
P.K. Buah-Busah, Laser and Fibre Optics Centre
University of Cape Coast, Cape Coast, Ghana

Needs for Optical Measurements in Combustion Processes or Energy Efficiency Improvement and Pollution Abatements
J.P. Martin, Paris, France

Contributed Paper
Aethalometer Applications for real time Monitoring of Combustion-derived Aerosol Carbon
F.A. Akeredolu, Obafemi Awolowo University, Ile-Ife, Nigeria
Dr. Len A. Barrie and Dr. Neil Trivett, Atmospheric Environment Service, 4905 Dufferin Street, Downsview Ontario, Canada

Optimization of Nox Removal by Non-thermal Plasma Discharge System
Yaw D. Yeboah, Zhicheng Wang and Kofi B. Bota,
Clarke Atlanta University, Georgia, USA.

OPTICAL DIAGNOSTICS

Invited Lecture
Optical techniques for diagnostics of combustion
P. Mazzinghi, INO, Istituto Nazionale di Ottica,
Firenze, Italy.

LASER TECHNIQUES IN COMBUSTION AND FLAMES

Invited Lecture
Principles of Laser Diagnostics for Combustion
P. Ewart, Oxford, U.K.

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Taieb Gasm, Unidad de Laser es, Instituto Pluridisciplinar Universidad compulsultense de Madrid, Madrid, Spain

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Dyson T. Jumpah, Environmental Protection Agency, Accra, Ghana

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Kwaw Anaman, Department of Mechanical Engineering, KNUST, Kumasi, Ghana
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PREFACE

This volume is a collection of invited papers, case studies and lectures presented at the ICS-UNIDO and University of Cape Coast Workshop on Combustion Diagnostics and Optical Techniques held from 5th July - 10th July, 1999 and hosted by the Laser and Fibre Optics Centre, Department of Physics at the University of Cape Coast, Cape Coast, Ghana and Coconut Grove Beach Resort, Elmina, Ghana. Lectures were held at the conference room of the hotel. ICS-UNIDO, through the effort of Prof. Gallieno Denardo in March 1998 has been able to bring together the academia and the industry through the organisation of this workshop. Such an initiative is first of its kind, in sub-Saharan Africa. This workshop was meant to encourage and entice industries to work in close association with Universities and Research Institutions. This workshop in Cape Coast, Ghana was organised as a follow-up to recommendations from the Expert Group Meeting held at Trieste, Italy from 1 - 5 June, 1998.

The workshop was able to bring together experts from Africa, Europe and USA to discuss pertinent issues on combustion systems. In addition the workshop focused on possibilities of transferring technical knowledge of relevance to the engineers and scientists from both Industries and the Universities as well as the Research Institutions. Considering the importance of combustion processes in energy production there was the need to transfer technological skills in various areas in combustion processes that are sensitive in solving the needs in the developing countries.

The workshop helped in creating awareness in combustion systems, and its associated problems, and the consequence of their emissions. It also provided the know-how of optical and imaging diagnostics of on-line monitoring of plant performance. It was realised during the sessions that there was the need to encourage the exchange of ideas between experts in developed and developing countries to be abreast with current trends.

It was also suggested that specific projects needed to be designed and planned to address the immediate needs of various industrial organisations. In addition, upcoming scientists and engineers were afforded the opportunity to interact with the experts invited to the workshop.

Experts from Ghana, Italy, France, United States of America and United Kingdom gave extensive and stimulating presentations on reviews and research findings on topics that probed from the introductory up to the advanced work in various fields to help solve problems relevant to industry, research and development.

- The main topics addressed were:
  - Air pollution due to combustion
  - Modelling of combustion diagnostics
  - Optical measurement methods
  - Emission and Absorption Spectroscopy
  - Laser induced Fluorescence
  - Laser Doppler Velocimetry and Laser probing of combustion
The workshop was able to identify issues such as the poor design of old domestic stoves and emissions from industries and vehicles that should be addressed. The assessment of emissions from stacks of smelters, oil refineries and industrial plants would indicate how much pollutants these industries give out daily to the populace for a healthy environment.

The workshop was well attended registering 60 participants and 10 lecturers including 20 graduate and undergraduate students from the University of Cape Coast (UCC) and Kwame Nkrumah University of Science and Technology, (KNUST) Kumasi.

The Regional distribution of participants and lecturers are as follows:

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In this volume, lectures from invited Lecturers as well as selected contributions from participants and case studies from industries have been included. Important issues which were brought to the fore to industrialists include:

a. good fuel formulation
b. Engine refinements
c. age of combustors and burners
d. flame characterisation and
e. efficiency in energy conversion through combustion design.

Readers would learn that optical techniques in monitoring combustion system require detail studies in some of the basic kinetics and theoretical modelling of flame characterisation.

I wish on behalf of the Advisory Board and Technical Committee of the workshop to express our indebtedness to Mr. W.S. Parker of Tema Oil Refinery Limited for his active involvement in soliciting for funds for this workshop;

Prof. G. Denardo for his initiative and involvement in promoting the organisation of the workshop as well as Ms. Vanier Vannessa for her secretarial abilities in coming out with initial preparation of document for the workshop.

My thanks are due to all local and foreign sponsors of this workshop. I am also grateful to all participants and lecturers who attended the workshop and in various ways contributed to its success.

Finally, thanks are due to Ms. Regina Eshun of Chemical Engineering Department, Kwame Nkrumah University of Science and Technology, Kumasi, Ghana for her marvellous job in organising and retyping the manuscripts as well as Ms. Doris Osei of Laser and Fibre Optics Centre, Ms. Mercy Yaadaar and Ms. Gertrude Quansah of Department of Physics, University of Cape Coast, Cape Coast, Ghana for their professional job of preparing this volume.


DR. F.K. BUAH-BASSUAH
LOCAL ORGANISER
FROM THE EDITORS

The workshop on Combustion Diagnostics and Optical Techniques which aimed at bringing together experts in Ghana and Europe, who are actively in the field of Combustion and Lasers, with representatives of industry, Research Institutions and Universities in Africa. The relevance in looking at the details of the processes in combustion and its consequent emissions have been identified.

Thanks to ICS - UNIDO initial support in organising this workshop, Tema Oil Refinery and other Oil Companies in Ghana made it possible to support the workshop and to come out with this volume of proceedings. The workshop which was organised by Laser and Fibre Optics Centre, Department of Physics, University of Cape Coast has now become a launching platform to start research activities in combustion related problems that are pertinent to some industries in the sub-region.

The workshop was directed by Mr. W. S. Parker, Prof. F. O. Akuffo, Dr. A. Brew-Hammond and Dr. P. K. Buah-Bassuah. It has become an important activity of ICS-UNIDO, South of Sahara to transfer technology to the doorsteps of industries in the sub-region. It was realised at this forum that much effort need to be used to monitor properly some emissions from our industries. It was a good opportunity for Scientists to interact with Engineers as a first step to solve common problems (such as means of checking emission of gases and to look into performance of old domestic stoves.)

The scientific programme of this workshop constituted seminars and Laboratory sessions. The report on the Laboratory sessions can be obtained from different report book

This volume contains fifteen (15) invited papers, five (5) contributed papers and five (5) case studies and also special addresses by invited dignitaries. These papers appearing in this manuscripts were read at the workshop and the necessary suggestions made during the discussions have been incorporated.

The papers have been arranged according to these themes

a). Combustion systems and Modelling
b) Monitoring process from combustion and its subsequent gaseous emissions.
c) Optical diagnostics and measurements
d) Laser techniques in combustion and flames

Under these broad headings are classified both the invited and contributed papers. At the end of this volume, is the evaluation of the workshop, communiqué, list of both lecturers and participants.

We appreciated very much the effort of the invited speakers, chairmen to all sessions, all the delegates, graduate and undergraduate student who kindly accepted our invitation and those who provided the manuscripts on time to enable us compile both the abstract and the proceedings.
We are most grateful to the staff and coordinator of ICS-UNIDO office especially Prof. G. Denardo and Ms. Varnier Vanessa for their fruitful contributions to this workshop. We greatly acknowledge Mr. P.K. Mensah of Laser and Fibre Optics Centre (LAFOC) for his enthusiasm in helping to prepare flyers, budget and first announcement of the workshop.

Once again, we are grateful to all those who contributed both materially and financially to make the workshop and the production of this proceedings a success.

Editors
PROGRAMME
PROGRAMME

SUNDAY, 4 July, 1999

09.00 – 12.00  Visit to Kakum Forest
12.00 – 14.00 Lunch Break
15.00 – 17.30 Visit to Elmina Castle

MONDAY, 5 July, 1999

08.00 – 08.50  Registration

09.00 – 10.30  OPENING CEREMONY
Conference Room, Coconut Grove Beach Resort
Chairman: Mr. W. S. Parker
Chief Executive, Tema Oil Refinery Limited (TOR)

08.50 – 09.00  Invited Guests seated at the Conference Hall

09.00 – 09.10  Introduction of Chairman and Invited Guest
Dr. P.K. Busuh-Bassuah
Local Organiser and Coordinator

09.10 – 09.20  Chairman’s response

09.20 – 09.30  Welcome Address: Prof. S.K. Adjepong
Vice Chancellor, University of Cape Coast, Cape Coast

09.30 – 09.40  Goodwill message, ICS – UNIDO

09.40 – 09.55  Short Address: Hon. Lt. Col. C.K. Agbenaza (rtd.)
Central Regional Minister

09.55 – 10.10  Short Address: Hon. Cletus Avoka
Minister of Environment, Science and Technology

10.10 – 10.25  Keynote Address: Hon. Ohene Kena
Minister of Mines and Energy

10.25 – 10.30  Chairman’s Closing Remarks

10.30 – 10.35  Vote of Thanks: Ms. Catherine Asante-Poku,
TOR, Tema

10.35 – 11.00  Coffee Break
Morning Session 1
Laboratory Session I
Visit to the Laser and Fibre Optics Centre by Dignitaries and Invited Guests.

13.00 – 14.30
Lunch Break

Afternoon Session I
Chairman: Mr. W.S. Parker
Chief Executive, TOR

14.30 – 15.30
LECTURE 1
Topic: Combustion Process, What is it?
Speaker: Prof. F. Akafo

15.30 – 16.30
LECTURE 2
Topic: Principles of Laser Diagnostics for Combustion
Speaker: Prof. P. Ewart

16.30 – 17.00
Coffee Break

Afternoon Session II
Chairman: Mr. J.P. Martin
Paris, France

17.00 – 18.00
LECTURE 3
Topic: Monitoring air pollutants with spectroscopic techniques
Speaker: Prof. P. Mazzinghi

19.00
Reception
VENUE: Vice Chancellor's Lodge
Vice Chancellor, University of Cape Coast
& Chief Executive of TOR to host
TUESDAY, 6 July, 1999

Morning Section II
Chairman: Prof. F.O. Akuffo
Dean, Sch. of Eng. KNUST, Kumasi

09.00 – 10.00
LECTURE 4
Topic: Application of Laser Diagnostics in Flames and Engines
Speaker: Prof. P. Ewart

10.00 – 11.00
LECTURE 5
Topic: Optical diagnostics of air pollutants
Speaker: Prof. P. Mazzinghi

11.00
Coffee Break

Morning Section III
Chairman: Prof. F.O. Akuffo
Dean, Sch. of Eng. KNUST, Kumasi

11.30 – 12.30
LECTURE 6
Topic: Advanced Measuring Techniques in Flames; Flow Field
And temperature measurements
Speaker: Prof. M. Mansour

12.30 – 14.00
Lunch Break

Afternoon Section III
Chairman: Prof. A. Ayensu
INSS, CSIR, Accra

14.30 – 15.00
LECTURE 7
Topic: Combustion modelling
Speaker: Dr. A. Brew Hammond

15.00 – 15.30
Coffee Break

15.30 – 18.30
Laboratory Session II

20.00
Conference Dinner
WEDNESDAY, 7 July, 1999

Morning Section IV
Chairman: Prof. Mazzinghi
INO, Firenze, Italy

09.00 - 10.00
LECTURE 8
Topic: Introduction to Turbulent Combustion
Speaker: Dr. D. Veynante

10.00 - 11.00
LECTURE 9
Topic: Monitoring air pollutants in combustion
Speaker: Dr. P.K. Buah-Basuah

11.00 - 11.30
Coffee Break

Morning Section V
Chairman: Dr. D.K. Dodoo
Dept. of Chemistry, University Of Cape Coast, Cape Coast

11.30 - 12.30
LECTURE 10
Topic: Needs for Optical Measurements in Combustion Processes for Energy Efficiency Improvement and Pollution Abatements
Speaker: Prof. J.P. Martia

12.30 - 14.00
Lunch Break

Afternoon Section III
Chairman: Dr. S.Y. Mensah
Head, Dept. of Physics, University of Cape Coast, Cape Coast

14.30 - 15.00
LECTURE 11
Topic: Advanced Measuring techniques in flames; major and Minor species concentration measurements,
Speaker: Prof. M. Mansour

15.00 - 15.30
Coffee Break

15.30 - 18.30
Laboratory Session III

20.00
Supper and Entertainment
THURSDAY, 8 JULY, 1999

05.00 – 16.30 Excursion to Tema and visit to Tema Oil Refinery (TOR) and Volta Aluminium Company (VALCO)

18.30 – 20.00 Dinner

FRIDAY, 9 July, 1999

Morning Section VI
Chairman: Dr. P.K. Buah-Bassuah
Local Organiser/Coordinator, LAFOC, University of Cape Coast, Cape Coast.

08.00 – 09.00 Round table conference (Resolution)

Morning Section VII
Chairman: Prof. Yaw Yeboah
Clarke Atlanta University, Atlanta, Georgia, USA

09.00 – 10.00 LECTURE 12
Topic: Turbulent Combustion Modelling:
- Classical Reynolds averaging approaches
- Large Eddy Simulations
Speaker: Dr. Veynante

10.00 – 11.15 LECTURE 13
Topic: (i) Improvement of the Modelling of Industrial Furnaces
And Processes following Experimental Observations
(ii) Analysis of Domestic Gas appliances for hot water
Production by Laser Induced Fluorescence and
Fourier Transform Emission Spectroscopy Measurements.
Speaker: Prof. J.P. Martin

11.15 – 11.30 Coffee Break
Morning Section VIII
Chairman: Dr. A. Owusu
Dept. of Physics, University of Cape Coast Cape Coast

11.30 – 12.30
CASE STUDY 1
Topic: Combustion processes in Oil Refinery
Speaker: Iag. K.K. Ditsa

12.30 – 13.00
LECTURE 14
Topic: CO₂ – Tea Laser-Based Lidar Dial system for the
Detection of hydrocarbon pollution in the atmosphere.
Speaker: Dr. Tsieb Gasmii

13.00 – 14.00
Lunch Break

Afternoon Section IV
Chairman: Prof. K. Yankson
Dean, Fac. of Science, University Of Cape Coast, Cape Coast

14.00 – 14.30
CASE STUDY 2
Topic: Combustion processes in thermal plant and Energy
Generation: Takoradi Thermal Power Plant
Speaker: Ing. Stephen K. Doku

14.30 – 15.00
CASE STUDY 3
Topic: Burner Controls in VALCO
Speaker: Mr. E.K. Avotri

15.00 – 15.30
Coffee Break

15.30 – 18.30
Laboratory Session IV

19.30
Dinner
SATURDAY, 10 July, 1999

Morning Section IX
Chairman: Mr. D.I. Lamptey
Head, Dept. of Agric. Engineering, University of Cape Coast, Cape Coast

LECTURE 15
08.00 – 09.00
Topic: Optimization of NOx Removal by Non-thermal Plasma Discharge System
Speaker: Prof. Yaw D. Yeboah

LECTURE 16
09.00 – 09.30
Speaker: Prof. Yaw Yeboah

LECTURE 17
10.00 – 10.30
Topic: Aethalometer Applications for real time Monitoring of Combustion-derived Aerosol Carbon
Speaker: Dr. F.A. Akedolu

10.30 – 11.00
Coffee Break

Morning Section X
Chairman: Mr. Brown Acquaye
Regional Fire Officer, Cape Coast

CASE STUDY 4
11.00 – 11.40
Topic: Combustion Processes Monitoring by the Environmental Protection Agency
Speaker: Mr. Dyson T. Jumpah

LECTURE 18
11.40 – 12.05
Topic: Laser Doppler Velocimetry and High-Speed Video Imaging for Combustion and Emission Control Research
Speaker: Prof. Yaw D. Yeboah

CASE STUDY 5
12.05 – 12.30
Topic: Pollutants from Combustion Systems of Automobile
Speaker: Mr. Kwaw Anaman
12.30 – 13.25  CLOSING CEREMONY
Prof. Kobina Yankson,
Dean, Faculty of Science,
University of Cape Coast, Cape Coast

12.30 – 12.35  Introduction of Chairman: Mr. Kofi Anane-Fenin
Dept. of Physics, University of Cape Coast
Cape Coast

12.35 – 12.40  Chairman’s remarks

12.40 – 12.50  Short Address and Communiqué
Dr. P.K. Buah-Bassah
Local Organiser/Coordinator, LAFOC

12.50 – 13.10  Guest Speaker: Mr. Tsatsu Tsikata
Chief Executive
Ghana National Petroleum Corporation, Tema

13.10 – 13.20  Chairman’s Closing Remarks

13.20 – 13.25  Vote of Thanks
Mr. P.K. Mensah
LAFOC, University of Cape Coast

13.30 – 14.30  Lunch

15.0  DEPARTURE
WELCOME ADDRESS

SPEECH DELIVERED BY PROF. S.K. ADIEPONG, VICE-CHANCELLOR AT THE ICS INTERNATIONAL WORKSHOP ON "COMBUSTION DIAGNOSTICS AND OPTICAL TECHNIQUES" HELD AT THE COCONUT GROVE HOTEL ON JULY 5, 1999.


It is a pleasure for me, this morning, to welcome you to this very important international workshop.

Coming on barely a month after the conference of the African Regional Council of the International Association of University Presidents held in Accra on the theme: "Forging Partnerships for Development", this workshop, which brings together the Universities and industry, is a very welcome manifestation of the expected collaboration between institutions of higher learning and industry. It is my expectation that this workshop will be a precursor to a closer and more intense collaboration between Ghanaian Universities and industry particularly in the examination of issues relating to science and technology and the environment.

Mr. Chairman, the volume of activities involving combustion and the environment pollution deriving therefrom has increased tremendously in this country in the last few years. The theme for this Workshop could not therefore have been better chosen. It is my hope that the workshop will give birth to a few research projects on
(a) Efficient monitoring of emissions using modern methods such as Laser techniques
(b) Plant performance of combustion systems for efficient energy conversion and the need to find solutions to pollution related problems.
I would like to suggest at this moment, to the industries to sponsor post-graduate research to enable Universities and research institutions to look into these problems. I would also recommend that some of the experiments set up to give hands-on-skills to participants should be developed into projects that could continue to address pollution problems in Ghana.

Mr. Chairman, Ladies and Gentlemen, permit me to commend and thank members of the workshop’s Local Organising Committee which worked so hard under the very active Chairmanship of Mr. W.S. Parker who demonstrated extraordinary commitment throughout the Committee’s work and who was personally responsible for raising most of the funds required for the Workshop. The committee comprised representatives from the Universities, Industry and Governmental agencies. It is my wish that the committee with its wide spectrum of membership would become a thematic group after the workshop and take on the responsibility of planning, overseeing and raising funds for the collaborative research that should necessarily be a product of this workshop.

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I would also like to thank all the companies, organisations and individuals who have contributed in cash or kind towards the successful organisation of the workshop. It is gratifying to note that they have not only given donations but they are participating in the workshop.

I have no doubt that the workshop will have a lot of focused activity and stimulating discussions. Indeed I expect participants to have a field day each day of the workshop. I wish you very fruitful deliberations as well as God's guidance and blessings.

Once again, I welcome you very warmly to this workshop.

Akwaaba!
CHAIRMAN’S OPENING REMARKS
BY W.S. PARKER CHIEF EXECUTIVE
TEMA OIL REFINERY (TOR) LTD.

Honorable Minister of Mines and Energy, Honorable Minister of Environment, Science
and Technology, Honorable Minister of Central Region, Your Excellencies, Members of the
Diplomatic Corp, the Vice-Chancellor of the University of Cape Coast, the Representative of the
International Centre for Science and Technology, Italy, Heads of Government Organisations and
Institutions, President of the Central Region House of Chiefs, Scientists, Engineers, Participants
and Lecturers of the workshop, Deans of Faculties, Students, Distinguished Ladies and Gentlemen.

I feel singularly honored for given me the opportunity to be a member of the organising
team for this Workshop and to be asked to chair this important opening session.

In April, 1997, I had a call from Prof. S.K. Adjepong, Vice Chancellor of the University
of Cape Coast who asked me to host Prof. G. Denardo from the International Centre for Science
and High Technology, Trieste, Italy. I had a fruitful discussion with him and he expressed an
interest in linking up activities of the Regional Laser and Fibre Optics Centre in Cape Coast and
Industries. As a first measure he asked me to nominate someone from Ghana to attend two expert
group meeting on Combustion which were held in Trieste on 1st – 5th June 1998 and 1st – 5th March
1999. At the first group meeting, in March 1998, Ghana was chosen to host this workshop.

I am pleased to say that the Workshop being held now in Cape Coast is the first of its
kind in Sub-Saharan Africa and we would like to thank ICS and UNIDO for providing
approximately $31,000 being 50% of the cost of the workshop. This was spent on foreign
participants and lectures. The remaining 50% of the cost has been provided locally by Stake
holders such as Tema Oil Refinery, Laser & Fibre Optics Centre, Kwan Nkrumah University of
Science & Technology, University of Cape Coast, Ghana National Petroleum Corporation, Volta
Aluminium Company Ltd., Volta River Authority, Ghana Oil Company Ltd. Mobil, Shell, Elf,
Total, Unipetro, Engen Petroleum Ltd, Tripc Oil Company, Allied Oil Company Ltd, Star Oil
Company Ltd., Ghana Automobile Distributors Association, Tema Power Company Ltd. and
Motherwell Bridge Ghana Ltd. We are extremely grateful for the concern and generosity of all
the donors.

I am delighted that we are here to have such an important workshop on Combustion
Diagnostics and Optical Techniques. We hope the organisers ICS-UNIDO will continue to link us
up to effectively interact with the Universities.

The basic combustion processes have been intensively studied for many years and a high
degree of optimisation has already been achieved. Further steps towards better efficiency and less
polluting combustion requires deeper understanding of all underlying chemical reactions and
physical processes which inevitably involve using highly advanced optical diagnostic techniques.
The continuous development of this research field in the industrialised countries is maintained by a

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number of important laboratories that rely on both governmental and industrial support which regrettably is lacking in our country at this moment except for this occasion. We need to consider this initiative here and help to achieve efficient and safe systems to enable us protect in a vigorous way our environment.

To a large extent, in the developing countries the situation is different. The main industrial technologies (including combustion) are normally imported. Thus, the key point is to develop local expertise in combustion control to ensure the correct operation of existing plants, as well as upgrading and retrofitting of old installations. These tasks are not simple at all and require qualified manpower.

It is on this note, that I will expect contributors of papers, and policy makers to exhaust various ideas to make our combustion process efficient and environmentally friendly.

We know the effect of pollutants on the environment which give rise to new by products which are injurious to human health. To fulfill the above mentioned objectives, there is the need to transfer technical know-how of relevance from the scientifically advance technologies to us for the efficient and sustainable management of industrial activities in this country.

Considering the importance of combustion processes in energy production and their technological aspects, we at this workshop should endeavor to press hard for the transfer of the technological know-how at the highest level in this field to up and coming Engineers and Scientists and create a general awareness of the effects of combustion processes on the environment.

I hope such a forum would assist industrialists, scientists and engineers to formulate policies to check our environment from degradation by using the most up to date monitoring techniques.

Thank you,
GOODWILL MESSAGE FROM ICS AND UNIDO

MESSAGE DELIVERED BY DR. MILTCHO DANAIOV
ON BEHALF OF GALLIENO DENARDO
ICS-ICTP LABORATORY FOR LASERS AND OPTICAL FIBRES
SYNCHROTRON RADIATION FACILITY, TRIESTE, ITALY

The subject of this course is part of a long term programme of the ICS-UNIDO. The aim is to promote co-operation between scientists working in academic institutions and technicians working in the industrial sector. Controlling combustion processes means driving physical and chemical phenomenon in such a way as to maximise the energy production/fuel consumption ratio and to minimize the environmental impact of the most common energy producing processes i.e. combustion of different fuels. These are motivations to appreciate the importance of the programme of this meeting.

The workshop is expected to stimulate the interest of scientists, technicians and industrial managers on the importance of expanding the research and training activities especially in techniques such as the use of laser based systems for combustion diagnostics.

We are confident that this workshop will enhance the interaction between industry and university so as to allow researchers to be informed on the practical needs of the production world and managers and technicians to be made aware of the most advanced views of science in order to innovate their own systems.

We look forward to hearing follow-up proposals of collaboration on specific cases so that this course should be just a step towards a long term programme.

I would like to convey my best wishes for a fruitful co-operation and congratulate the organisers particularly Dr. Paul Buah-Bassuah and Prof. S.K. Adjepong on their continuing work aiming at enhancing science and technology programme in our beloved Ghana.
SHORT ADDRESS

SPEECH DELIVERED BY HON. LT. COL. C.K. AGBENAÑA (RTD), MP
CENTRAL REGIONAL MINISTER,
AT THE ICS INTERNATIONAL WORKSHOP
ON COMBUSTION DIAGNOSTICS AND OPTICAL TECHNIQUES

Mr. Chairman, Honorable Minister of Mines and Energy, Honorable Minister of Environment, Science and Technology, Your Excellencies, Members of Diplomatic Corps, The Vice Chancellor of the University of Cape Coast, The Representative of the International Centre for Science and Technology, Italy, Heads of Government Organisations and Institutions, President of Central Region House of Chiefs, Scientists, Engineers, Participants and Lecturers of the workshop, Deans of Faculties, Students, Distinguished Ladies and Gentlemen.

I feel very honoured to be associated with this workshop which holds a lot of promise for Energy, science and technology for this Region. As you may be aware this Region, and in particular Cape Coast, has been the focal point for the development of education in the country and at the same the place to commemorate the celebration of PANAFEST. This workshop no doubt is of much relevance to us.

I am grateful for the opportunity offered by the workshop organizers to get me connected with the activities of the Regional Laser and Fibre Optics Centre of the University of Cape Coast. I am reliably informed that the combustion diagnostics and optical techniques, which are the theme of the workshop tends to look at useful utilization of Energy without polluting the environment with emission. I also noted that the workshop is aiming at transferring hands on skills to participants to diagnose and monitor the performance of plants in site.

Mr. Chairman, ladies and gentlemen, my information is that Combustion processes per se, include small and large scale reactors, steady and unsteady processes, atmospheric as well as pressurised units, representing all kinds of industrial equipment from large furnaces in power generating plants, to small in-house burner for heating, etc. The area of coverage of combustion processes in our socio economic development is quite enormous and essential, however, in developing countries such as ours the main industrial technologies are normally imported. It is very necessary to develop local expertise in combustion control for standard operation of the already existing plants as well as for upgrading and retrofit of old installations. These tasks are not simple at all and require qualified manpower. Any under-estimation of this fact have tragic consequences, as demonstrated by several recent accidents in power plants in our sub-region.

It is my hope that Scientists and Engineers at this important workshop would come out with useful techniques acquired from your deliberations to better the lot of the average Ghanaian. I also hope that you would intensify your efforts to have a deeper understanding underlying combustion systems using the highly developed Laser Techniques since the laser-based diagnostic methods are indispensable tools.
Mr. Chairman, although the Central Region has not yet seen much of the effect of pollution from combustion process, I wish to recommend that serious monitoring of pollutants and examination of combustors should be initiated to bring awareness of the problem to our people.

I will also entreat the Energy Board to institute research activities into combustion process and to ensure the switch over from total dependence on biomass to LPG gas for our domestic usage. I will caution against the frequent use of oil lamps in selling kenkey which tends to produce soot that adversely affect human life. I believe through research the reduction of PAH and other emissions from kerosene stoves to oil lamps can also increase the life expectancy of our women.

Mr. Chairman, before I resume seat I wish to once more commend all those who in diverse ways have contributed to the smooth organisation of this workshop and wish you a fruitful stay in the region. Special mention must be made of Prof. S.K. Adjepong, the Vice Chancellor of the University of Cape Coast in particular and Mr. W.S. Parker of Tema Oil Refinery Limited for hosting this workshop. I hope such workshops would become a regular feature to regulate combustion processes in the country.

I thank you very much for your attention.

Thank you.
SHORT ADDRESS

SPEECH DELIVERED BY
HON. MR. CLETUS A. AVOKA (MP),
MINISTER OF ENVIRONMENT, SCIENCE AND TECHNOLOGY
AT THE INTERNATIONAL WORKSHOP ON COMBUSTION DIAGNOSTICS
AND OPTICAL TECHNIQUES 5TH-10TH JULY, 1999.

Mr. Chairman, Colleague Ministers of state, Vice Chancellor, University of Cape Coast,
Members of the Diplomatic Corps, the Representative of the International Centre for Science and
high Technology, (ICS) Trieste, Nanom, Distinguished Science and Engineers, invited Guests,
Ladies and Gentlemen.

I have the greatest pleasure to be associated with this international workshop being
organized by International Centre of Science and High Technology (ICS), Trieste, the United
Nations Industrial Development Organization (UNIDO), and the Laser and Fibre Optics Centre,
University of Cape Coast, under the theme “Combustion Diagnostics and Optical Techniques.

Mr. Chairman, one of the major problems facing the global community at the moment
relates to global warming, which is associated with the release into the atmosphere of greenhouse
gases. The major sources of these greenhouse gases are transportation, industrial processes or
household cooking.

The Climate Change Convention provides the framework within which the global
community is to take measures to reduce the quantities of these gases currently being emitted into
the atmosphere. All parties to the Convention, including Ghana, are expected to put in place to
reduce the levels of these greenhouse gases.

To us at the Ministry of Environment, Science and Technology, therefore, organising this
workshop at this time seems very opportune. This is because under the National Climate Change
Committee, efforts are being made for the country to evolve its strategies for the implementation
of the Climate Change Convention. Though as a country our various developmental activities may
not be generating appreciable amounts of greenhouse gases to affect the global climate, economic
considerations at least make it imperative for us to introduce measures to improve combustion
efficiency to enhance proper utilization of our energy resources and thus reduce the quantities of
greenhouse gases generated by our experts to interact with their colleagues from other countries on
how to diagnose the problems associated with combustion and this find ways in which to reduce
the emissions arising from combustion.

One important setback in the country’s efforts to manage its environment in general is the
lack of facilities to monitor the level of emissions and pollutants from the various economic
activities. It is appreciated that most of these equipments tend to be expensive. Individual institutions may thus not be in a position to acquire on their own. There is thus the need for the pooling of resources in this effort. I am thus happy to see this initiative by the International Centre for Science and High Technology which when operational will make it possible for the Laser and Fibre Optics Centre of the University of Cape Coast to offer technical assistance to our industries in their efforts to improve upon the efficiency of their operations.

I wish to take this opportunity to inform participants that as part of the measures that the Ministry of Environment, Science and Technology is taking to reduce the emissions arising from transportation, the Environmental Protection Agency has recently make available to the Vehicle Examination and Licensing Division of the Ministry of Roads and Transport equipment to monitor emissions from vehicles.

This action together with the initiative by the International Centre for Science and High Technology for the Laser and Fibre Optics Centre should help his country in building the capacity for assessing air pollutants and thus help the country meet its obligations under the Climate Change Convention.

Distinguished Scientists, as we consider how to monitor the levels of air pollutants arising from the various economic activities, it is important for us to remember the saying that “Prevention is better than cure”. It is not possible to introduce for use in this country fuels which do not generate as much greenhouse gases as those currently in use in this country. A number of countries are currently using ethanol and methanol as fuel for vehicles. Ethanol can also be blended with kerosene for use as fuel in kerosene stoves. I will like our scientists to look at the implications of these technologies and provide us, policy makers, with the cost benefit analysts for their use in the country.

Mr. Chairman, one other important objective of this Workshop is “to promote closer links between industries and research institutions”. This is an issue which my Ministry is pursuing very seriously as part of its programme of ensuring that the research and development institutions in the country meet the needs of the private sector. At the launching of the celebrations of this year’s Day of Scientific Renaissance of Africa, I proposed the establishment of Research-Industry body to promote this link. I will like participants at this Workshop to deliberate on this issue and provide my Ministry with some concrete proposals on how this is to be achieved.

Distinguished Workshop Participants, even though this Workshop is not directly addressing climate change issues, I believe that my comments have drawn your attention to the impact of combustion on climate change. It is my hope that after this Workshop, the local participants will join my Ministry in our efforts at implementing the Climate Change convention in the country. I will also like to see greater co-operation between our research and academic institutions on how to help the local industries to solve their various problems which adversely affect the environment.

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Mr. Chairman, Ladies and Gentlemen, let me end my short address by expressing my gratitude to the organisers of this Workshop for recognizing its importance to the Ministry of Environment, Science and Technology. It is my hope that the scientific and technological discussions over the next few days will help in improving the environment in which we are living. I will be interested in the outcome of your Round Table Conference when a resolution is to be made.

I wish you all the best in your deliberations.

Thank you and may God bless you all.
KEYNOTE ADDRESS
DELIVERED BY HON. FRED OHENE-KENA
MINISTER OF MINES & ENERGY
AT THE OPENING OF A WORKSHOP ON “COMBUSTION DIAGNOSTICS AND OPTICAL TECHNIQUES”
CAPE COAST, 5 – 10 JULY, 1999

Mr. Chairman, Hon. Minister of Environment, Science and Technology, Hon. Regional Minister, Your Excellency, Members of the Diplomatic Corps, President of Central Regional House of Chiefs. The Vice Chancellor of the University of Cape Coast, The Representative of International Centre for Science and Technology, Italy, Heads of Government Organizations and Institutions, Scientists, Engineers, Students, Distinguished Ladies & Gentlemen.

It is with great pleasure that I am present with you at the opening of this International Workshop on the theme: “Combustion Diagnostics and Optical Techniques”. This workshop is unique in the sense that, it is an attempt to foster closer interaction between Industry and the Universities to find solutions to environmental problems associated with combustion. I am really delighted to note that it is an initiative from the United Nations Industrial Development Organization (UNIDO) to transfer technology to Developing Countries. Though UNIDO has been undertaking such projects in North Africa, it is the first time such an activity is being organized in sub-Saharan Africa. Taking a look at the attached programme, I realize that the workshop consists of both seminars and practical sessions and is intended to expose participants to current activities on, and future prospects of Laser and Optical techniques in Combustion processes.

It is gratifying to note that the topics to be discussed include Air pollution due to combustion, modelling of combustion diagnostics, optical measurement methods, Emission and Absorption spectroscopy, and the various techniques for the Probing of combustion. The use of Lasers in environmental monitoring is also to be emphasized. In addition, various experiments have been mounted to give hands-on training to participants and open up some new ideas in understanding the dynamics and efficient utilization of flames.

Despite the increasing use of alternative energy sources, the burning of fossil fuels and biomass, results in the emission of carbon dioxide (CO₂) the most abundant global warming gas, and other pollutant species like the oxides of Sulphur (SO₂) and Nitrogen (NOₓ). These and other particulate matter (PM) such as soot and Poly-aromatic hydrocarbons are rarely monitored in developing countries.

In Ghana, the major source of hydrocarbon, oxides of nitrogen and sulphur from combustion processes are the petroleum refining plant and the numerous marketing outlets of petroleum products. Vehicular transport also contributes to oxides of nitrogen into the atmosphere. The effects of such combustion processes on human beings are enormous. Ongoing research indicates that emissions from wood burning in the rural areas tend to affect the eyes of rural folks. Heat and high temperatures from combustion furnaces are possible means of affecting human health thereby reducing efficiency. It is sad to note that the fundamental problem of all industries and mining areas in Ghana is lack of equipment to monitor gas releases.

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Unfortunately, the point source of emission of these pollutants from refinery as well as those of steel and aluminium smelters for example may be many feet above the ground or not easily accessible with the traditional monitoring techniques.

It is gratifying to note that this workshop is going to give us the awareness to help our scientists and technologists adapt and improve on their research methods and to assist our industries and mines, whose activities impact negatively on human life to operate in an environmentally friendly manner.

Mr. Chairman, it is known that the pollutants from combustion processes such as domestic stoves, industrial burners and internal combustion engines can be reduced by optimizing air-fuel ratio, flame temperature and mixture formation system. Industries in Ghana lack monitoring instruments and automatic air-fuel ratio controlling devices. As a result, boilers are not operating at optimum air-fuel ratio which means energy is lost and pollutants are excessively emitted.

It has been established that simple domestic stoves cause high emission of poly aromatic hydrocarbon and carbon monoxide, which contribute to the reduction of life expectancy in developing countries. There are standards on emissions but not on burners and combustors. Vehicular emissions and those from domestic burners make the environment appear darker.

My Ministry and that of Environment, Science and Technology have therefore taken cognizance of these problems and I would like the workshop to come out with some modalities to regulate pollution from combustion systems in the country.

At this point Mr. Chairman, I want to recognize the roles of the Environmental Protection Agency in their monitoring programmes to quantify emission levels for the reduction of energy consumption and for the protection of the environment. However, I will implore them to further increase their efforts to measure combustion emissions from vehicles, domestic stoves and industrial burners.

In addition my Ministry is still concerned with improved stoves design and the need to accelerate the shift to the use of LPG Gas stoves to save our environment.

It is a welcome news that the workshop will be exploring the use of laser techniques as a possible alternative for the detection, prevention and monitoring of gases, from combustion systems for higher efficiency and good performance. Optical diagnostics induces minimal disturbance to a system and pursues non-contact probing, providing information with high sensitivity and selectivity.

Mr. Chairman, I would urge the Energy Commission, in collaboration with Laser and Fibre Optics Centre of University of Cape Coast and Mechanical Engineering Department of Kwame Nkrumah University of Science and Technology, to come out with research programmes
aimed at enhancing reduction in emissions and improving performance of our industrial combustion. A research work such as quantifying combustion emission levels, for instance, will be very important for the formulation of policies on emission regulation.

Mr. Chairman, permit me now to express my appreciation, to the Director, Prof. G. Denardo of International Centre for Science and Technology of UNIDO, for initiating such a project in Ghana. I also wish to thank the Office of External activities of the International Centre for Theoretical Physics, for establishing the Regional Laser Centre at Cape Coast and supporting it with funds and equipment for the promotion of the new technology in Ghana, I understand that the centre is engaged in other research works for the promotion of agriculture and communication.

Due recognition and appreciation also go to Mr. W.S. Parker, Chief Executive of Tema Oil Refinery for helping in the organization of this workshop as well as providing some equipment for the smooth operation of the laboratory sessions. Finally, my congratulations go to the Chairman of the Ghana atomic Energy Commission (GAEC), Prof. F.K.A. Allotey and the Vice-Chancellor of the University of Cape Coast, Prof. S.K. Adjepong on their foresight in initiating steps for the establishment of the Regional Laser and Fibre Optics Centre in Ghana.

It is now my singular honour to declare the Workshop on Combustion Diagnostics and Optical techniques formally opened.
CHAIRMAN'S CLOSING REMARKS
BY W.S. PARKER CHIEF EXECUTIVE, TEMO OIL REFINERY

Honourable Minister of Mines and Energy, Honourable Minister of Environment, Science and Technology, Honourable Central Regional Minister, Your Excellencies, Members of Diplomatic Corps, the Vice-Chancellor of the University of Cape Coast, the Representative of the International Centre for Science and Technology, Italy, Heads of Government Organization and Institutions, President of Central Region House of Chiefs, Scientists, Engineers, Participants and Lecturers of the workshop, Deans of Faculties, Students, Distinguished Ladies and Gentlemen.

I presume this morning's proceedings have been very worthwhile and I should like to give some comments on some observations I made during the speeches delivered by our August speakers.

It is quite interesting to note that this workshop has opened the floodgates for better and cordial relations between Industries and Universities. This Vice Chancellor in his welcome address has reiterated that concrete project should be established whereby graduate students would be taken to do some studies into common problems pertinent to the industry and society. He is aiming towards industrialization that will require a class of experts in this country to use modern technology to fulfill our needs and to seek also redress to a number derived from combustion system and its gas emission that bring along a number of problems of cultural and environmental decent.

In the keynote address, the Minister of Mines and Energy informed us that Combustion systems is dictated by fuel formulation, engine refinements, age of combustors and burners, flame characterisation and efficiency in energy conversion. The success of any industry requires the fulfillment of the above parameters to make plant performance well and give minimum pollutants. He put up query that monitoring is almost absent in our industries due to lack of equipment. I will implore the Environmental Protection agency to look into this and initiate a research work to help improve energy conversion and minimization of pollutants so as to help improve life expectancy of our people. He also asked us to formulate point projects whose results could be incorporated in policy formulation on emission regulation. He also encouraged Laser and Fibre Optics Centre (LAFOC) and research institutions to concentrate on capacity building to feed our upcoming industries and other sensitive areas of our economy. Above all, the Minister was our Engineering Departments to improve on the stove design on our homes to give less pollutants.

The Minister of Environment, Science and Technology commended TOR for undertaking major retrofit of its furnaces and heat exchange systems for optimizing combustion process to improve efficiency and reduction in emission of gases. We therefore want to encourage prevention of emissions and efficient energy conversions. It was interesting to note that most of our cars and trucks are aged and give emissions. Our stoves do give pollutants because of lack of proper fuel blending. It is a challenge to our oil industries to think about it.

The Ministry hopes to see the use of Laser techniques help solve most of these problems.
The Central Regional Minister advised that our women should be helped by having environmental friendly stoves to beat down pollution. He was of the opinion that there should be a shift from the use of biomass to LPG to conserve our forest. He therefore request that the Energy Board, Laser and Fibre Optics Centre (LAFOC) and the research institutions should work hard to come out with proper solutions to such problems.

I think the case studies to be presented by Industries and Mines as well as contributors of Scientific papers would help us come out with policies that enable us improve on the performance of our industries and help check environmental pollution.

I wish you all a successful workshop.

Thank you.
CHAIRMAN'S OPENING REMARKS
DELIVERED BY PROF. KOBINA YANKSON,
DEAN, FACULTY OF SCIENCE, UNIVERSITY OF CAPE COAST AT
THE CLOSING CEREMONY OF WORKSHOP ON COMBUSTION DIAGNOSTICS
AND OPTICAL TECHNIQUES 10TH JULY, 1999.

The Chief Executive, Mr. Tsatsu Tsikata, the Representative of the International Centre
for Science and High Technology, Heads of Government Organisations, Scientists, Engineers,
Participants and Lecturers of the workshop, Deans of Faculties, Students, Distinguished Ladies
And Gentlemen.

It is my greatest pleasure to be chairing this important function which is meant to bring
down the curtain on the International Workshop on Combustion Diagnostics and Optical
Techniques.

Though the workshop looked at very important themes and issues, I presume that it
concentrated on current activities of most industries in combustion systems and also looked at
future prospects of using Laser and Optical Physics in monitoring gaseous emissions and optical
techniques in the applied research.

This forum has done well to bring together, policy makers, experts from industries and
academicians to realise the essence in fostering collaboration in need-driven projects for both
industries and the public.

We are aware that lack of adequate equipment has rendered ineffective monitoring of
some gaseous emissions released in this country and probably elsewhere in West Africa. I believe
strongly that local capacity building in Laser technology would, enable us include the laser-based
techniques in our efforts to solve the pollution problems that arise from industrial activities.

I therefore see this workshop as an important milestone for my faculty and the laser
centre for improving the living standards of the people in the country. The linkages being sought at
this workshop will even push us further ahead.

Mr. Guest Speaker and Distinguished Ladies and Gentlemen, we hope to see a new era
where research results will satisfy the needs of industry thanks to the outcome of this workshop.

I hereby seek your co-operation and efforts in steering the affairs of this function.

Thank you.
SHORT ADDRESS

BY DR. P.K. BUAH-BASSUAH, COORDINATOR, LASER AND FIBRE OPTICS CENTRE, (LAFOC) UNIVERSITY OF CAPE COAST AT THE CLOSING CEREMONY

Mr. Guest Speaker, Mr. Chairman, Scientists, Engineers, Environmentalists Distinguished Ladies and Gentlemen, the International Workshop on Combustion Diagnostics and Optical Techniques was organised to close up the gap between the industries and the academia.

We have been made aware at this workshop that to effectively transfer technical knowledge of relevant scientific based technology for an efficient and sustainable management of industrial activities we need to:

1. develop experiments that could be user-oriented and present immediate benefits to the country
2. design projects that should foster proper linkages between the industries, Universities and research institutions
3. Make use of the projects to give technical skills through on-the-job training of personnel from both industries and universities.

The Laser and Fibre Optics Centre (LAFOC), which is seeking assistance for equipment to do some research work in fields such as engineering and industry, agriculture, communications and environmental monitoring e.g. to large extent has won the support of some international organisations such ICS-UNIDO and laboratories in Firenze, Italy in:

1. establishing laser-based optical systems to monitor industrial activities.
2. acquiring equipments from external funding agencies to initiate postgraduate training to satisfy the manpower needs of the industries.
3. fostering contacts with laboratories in Europe to develop environmental monitoring projects

I am happy to say that after realising the need and various role combustion systems play in solving most energy problems, the Centre has now the confidence to look for greater participation of projects from the industries to achieve the desired goals and to satisfy the manpower needs of the country for the economic and social needs of the people in this country. We have realised that meaningful work could be achieved through institutional collaboration and interdisciplinary share of ideas since the problems to be addressed are essentially of local nature and in addition require some local funding from both private and public sectors.

Mr. Chairman, I am pleased to state that LAFOC is now full grown to undertake research work which will benefit the industries and public at large as well as postgraduate training in this field. I will do my best to use all the facilities of the Centre and awareness created in this workshop to the professionals to experience the potentialities of the new developments of the
Laser technology. Now is the time laser-based measurement of combustion originated pollution is going to be done without disturbing the operations of our industries.

Finally, I am most grateful to all the funding agencies for their involvement in the organisations of this workshop.

Thank you and God bless you all.
GUEST SPEAKER'S ADDRESS

DELIVERED BY MR. TSATU TSIKATA, CHIEF EXECUTIVE GHANA NATIONAL PETROLEUM CORPORATION AT THE CLOSING CEREMONY OF THE WORKSHOP ON COMBUSTION DIAGNOSTICS AND OPTICAL TECHNIQUES ON SATURDAY 11TH JULY, 1999

Mr. Chairman, Distinguished Guests, Distinguished Resource Persons and Participants in the Workshop, Ladies and Gentlemen,

It is a pleasure to join you at this closing ceremony for the International Workshop on Combustion Diagnostics and Optical Techniques. This Workshop is another manifestation of the continued collaboration between the University of Cape Coast and the ICS-UNIDO. I have no doubt that both institutions have much to gain from such collaboration: the University is able to participate in scientific research at the highest international level and, appropriately, to provide a venue for scientists and practitioners of science in industry in this part of the world to share such knowledge and to exchange ideas and experiences. For the ICS also, I am sure a workshop like this provides an excellent opportunity both for diffusing the results of their researches and for obtaining valuable feedback which will enable new angles of research to be formulated and some new directions in ongoing work to be evolved.

Those of you who have taken part in this workshop have undoubtedly been realizing the fruits of this collaboration but it will not be enough to keep these benefits to yourselves. It is my expectation that you in turn will diffuse the knowledge into the environment from which you have come to this workshop and thus deepen the commitment to such international scientific collaboration of those under whose auspices you came.

It is gratifying to note that several participants are involved in industries which stand to benefit from the important scientific research work you have been exposed to. I am also pleased that Tema Oil Refinery and its Chief Executive, who chaired the Organising Committee, have been so active in their support for this workshop. We in the Ghana National Petroleum Corporation have been supportive for many years of Workshops like this involving the ICS because of our firm conviction that our societies must be active participants in scientific culture, which is a heritage of mankind and not the preserve of any part of the world. It is valuable to the work of our Corporation that such close links should exist between research institutions and industry and I would like to assure the University that we will continue to work closely and also help encourage other industries to be part of this important collaborative effort.

The history of science teaches us clearly that scientists have taken as fundamental starting points basic and simple life experiences, commonplace phenomena and sought to deepen their understanding of the world around them. I do not think that scientists working in Africa, for instance, can spurn their own surroundings and imagine that they will develop their scientific understanding by simply relying on the experiences of others living in different environments. The challenge of science is surely the opening of our eyes and minds to what is close by us. I am
therefore pleased to learn that your work this week has paid attention to realities around us such as the use of kerosene stoves and oil lamps and how the pollutants from these implements affect the eye.

One of the projects that our Corporation has been very committed to is that of promoting the transformation of domestic energy use away from woodfuel to more environmentally satisfactory solutions such liquefied petroleum gas. We have designed cook stoves based on the traditional ‘bukyia’ after we undertook surveys in various communities to understand cooking habits. One of the observations we also made was the adverse impact of cooking by firewood on the eyes of the women who do the cooking. Sometimes male scientists miss these realities because they are not involved in the cooking - they just wait for the cooked food! - and therefore do not pay attention to the obvious health hazards. If this Workshop has made you more sensitive to the daily experiences of food sellers in the night markets, for instance, or of people sleeping in bedrooms with lanterns emitting soot all night, I think it has achieved a lot. From such revelations many scientific insights are waiting to be unearthed!

I believe it is also timely that this workshop comes at a time when the importance of natural gas fired energy generation has become obvious throughout the world and specifically in our country where we have experienced a serious shortfall in energy from dependence on hydro-electric power. The value of natural gas as a clean and efficient fuel is well known, but perhaps just as the Regional Laser Centre was able to mount experiments on combustion process for participants at the workshop to undertake some measurements, it will be valuable for the Centre to measure emission levels from various fuels being used for thermal generation so that scientific evidence can affect policy decisions about choice of fuel as we enter a new era of increasing thermal power generation. This will not only be of value in Ghana but for the whole of the West African sub-region and Africa as a whole as various projects are being undertaken to address energy shortfalls and thus contribute to our development efforts. In neighbouring Nigeria we all know how billions of cubic feet of natural gas are flared every day in association with oil production. We need to monitor effectively activities of the oil industry and transform these emissions into energy for the people of this sub-region.

Assessment of emissions from stacks of smelters, oil refineries and power plants will assist the work of the Environmental Protection Agency in assessing environmental impacts from various combustion processes. The experiences of this workshop should therefore be able to contribute immensely to our development path not only in Ghana but throughout the continent of Africa. But this will not be an easy process; again, the history of science teaches us that scientific truths are often resisted by a barrage of prejudices, assumptions, deeply held beliefs, that are not easily shaken off, but we must pile on relentlessly the empirical evidence backing the scientific truth we seek to project in order to let it sink in.

Let me make a final observation. The growing gap between rich and poor countries in the world, as has been acknowledged, is reflected in the science and technology gap exist between the various countries. Yet we know that developing countries also have produced scientists of immense stature such as Prof. Abdus Salaam, the brain behind the ICS. We know that in countries
like ours, in institutions like the UCC, there are many brilliant scientific minds who are a match for scientists in a developed world. If the science and technology gap is to be bridged, it will be through the dedicated and energetic efforts of people such as you who have participated in this workshop and those with whom you will share the knowledge you have gained to influence your societies with such knowledge. This will also require that we give credence to expertise within our midst and not wait for our own experts to be validated by a foreign source before acknowledging the value of their expertise. All of us have a vital role to play in this growth in our scientific capacities and in the growth in confidence in our abilities to transform unacceptable conditions of under development to improvements rooted in growing knowledge of realistics around us - which is what science is about.

I thank you for your attention.
CHAIRMAN'S CLOSING REMARKS

BY PROF. KOBINA YANKSON, DEAN, FACULTY OF SCIENCE,
UNIVERSITY OF CAPE COAST

The Chief Executive, Mr. Tsatsu Tsikata, the Representative of the International Centre for Science and High Technology, Heads of Government Organisations, Scientists, Engineers, Participants and Lecturers of the workshop, Deans of Faculties, Students, Distinguished Ladies And Gentlemen.

We have been fortunate to have a successful workshop for the past week to deliberate on very important issues that apply to combustion systems and its practical applications as well as the consequences of the emissions that arise from these activities.

I have noted here that from the Guest Speakers speech there are a lot of problems that need immediate solution to improve on the living standards of our rural folks. For instance why do we still use kerosene stoves, oil lamp and lanterns in our daily activities as we are aware of their pollution effects. Scientists and Engineers are challenged to come up with new methods to design alternate means of enhancing clean use of energy.

The Guest Speaker would like to see a proper linkage in the research efforts between the industry and the Universities. Collaborative research is being called for instead of individualistic approaches which tend to be time consuming and not cost effective.

Follow-up activities of this workshop will promote cleaner use of energy and proper monitoring of the gaseous emissions using laser-based techniques.

I hope the skills acquired by the participants at this workshop will be properly used at their various places of work whilst the case studies presented could be turned into meaningful projects as well.

Congratulations to everybody for a good work well done.

I wish all the participants and lecturers a safe journey back home.

Thank you.
SCIENTIFIC SECTIONS & PRESENTATIONS

COMBUSTION SYSTEMS AND MODELLING
COMBUSTION: WHAT IS IT?

Fred O. Akuffo
Department of Mechanical Engineering
University of Science and Technology,
Kumasi, Ghana

ABSTRACT
The purpose of the presentation is to survey the basic principles that are needed to analyse and appreciate various combustion phenomena as well as their applications in key economic activities. The topics include properties of common fuels, air requirements, energy released by combustion, combustion in automobile and stationary power generation engines, combustion products and air pollution and emission of Green House Gases (GHG) from combustion processes in various sectors of the Ghanaian economy.

1.0 INTRODUCTION: Combustion defined
Combustion refers to the relatively fast, chemical reaction, usually accompanied by a flame, which occurs between a fuel and oxygen, or an oxygen carrier, that releases substantial quantities of energy as heat. Engineering applications of combustion are shown in Fig. 1.

During the process, the molecular bonds, or chemical bonds, between the reactant molecules are broken down and the molecules recombined to form new products that differ chemically from the original reactants. The internal, chemical or potential energy of the products is lower than that of the reactants and the difference in internal energy is released as heat to the surroundings or environment through the combustion products.

The physics and chemistry of the combustion process - breakdown and re-arrangement of molecules with subsequent release of energy as heat - require very high local temperatures (1620-2000 °C) and they occur within a few millionths of a second and within a characteristic length of a few angstroms i.e. means free path.

Therefore investigation of the microscopic aspects can only be done using high speed computers and relevant optical techniques including lasers. These difficulties have impeded major progress in engineering applications, particularly improving the efficiency of high speed internal combustion engines.

2.0 FUELS
A fuel is a material that can be burned to release energy. Most common fuels consist primarily of hydrogen and carbon and they are called hydrocarbon fuels and denoted by the general chemical formula C_nH_m. Hydrocarbon fuels exist in all phases, some examples being coal, (solid) gasoline (liquid) and natural gas (gaseous). The fuels normally used are derived from the distillation of crude petroleum. At TOR, this process usually yields kerosene (domestic and aviatian fuel), heavy gas oil, light gas oil; heavy gasoline or naptha, LPG and fuel gas.
In Ghana, as in many developing countries, woodfuels constitute the main source of energy contributing nearly 69% of total energy consumption. The woodfuel and its derivative charcoal are used mainly for cooking in both the urban and rural areas.

2.1 SOLID FUELS

Table 1 shows typical properties of coal, including its composition. For solid and liquid fuels, the analysis is quoted as a percentage by mass of each chemical element in the fuel and it is termed an ultimate analysis. A proximate or fixed carbon analysis may also be used for engineering considerations.

<table>
<thead>
<tr>
<th>Coal</th>
<th>C</th>
<th>H</th>
<th>O</th>
<th>N + S</th>
<th>Ash</th>
</tr>
</thead>
<tbody>
<tr>
<td>Anthracite</td>
<td>90.27</td>
<td>3.00</td>
<td>2.32</td>
<td>1.44</td>
<td>2.97</td>
</tr>
<tr>
<td>Bituminous</td>
<td>74.00</td>
<td>5.98</td>
<td>13.61</td>
<td>2.26</td>
<td>4.75</td>
</tr>
<tr>
<td>Lignite</td>
<td>56.52</td>
<td>5.72</td>
<td>31.89</td>
<td>1.62</td>
<td>4.25</td>
</tr>
</tbody>
</table>

2.2 LIQUID FUELS

Petroleum oils are complex mixtures of a large number of hydrocarbons. The most common being paraffins (C<sub>n</sub>H<sub>2n+2</sub>), olefins and naphthenes (C<sub>n</sub>H<sub>2n</sub>) and aromatics. The ultimate analyses are very similar and the choice of fuel for a particular application depends mainly on other characteristics such as viscosity, ignition temperature, knocking tendency (petrol engines) and cooking tendency (gas turbines).

2.3 GASEOUS FUELS

A few hydrocarbon fuels occur naturally as gas under normal conditions of temperature and pressure except Methane (a paraffin, C<sub>4</sub>H<sub>8</sub>) called natural gas.

Table 3 summarises properties of some gaseous fuels.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Methane</td>
<td>16</td>
<td>7.9</td>
<td>1.26</td>
<td>2.44</td>
</tr>
<tr>
<td>Ethane</td>
<td>30</td>
<td>8.0</td>
<td>2.40</td>
<td>4.99</td>
</tr>
<tr>
<td>Propane</td>
<td>44</td>
<td>37.8</td>
<td>16.63</td>
<td>35.13</td>
</tr>
<tr>
<td>1-Butane</td>
<td>58</td>
<td>19.0</td>
<td>11.02</td>
<td>23.54</td>
</tr>
<tr>
<td>n-Butane</td>
<td>58</td>
<td>27.3</td>
<td>15.83</td>
<td>33.87</td>
</tr>
<tr>
<td>Total</td>
<td>100.0</td>
<td>47.14 (MW)</td>
<td>100.00</td>
<td></td>
</tr>
</tbody>
</table>

CONCLUSIONS
1. The energy sector contributed 16% of the total GHGs in Ghana in 1990, second to agriculture which contributed 79%. Industry contributed only 1.6%.

2. Within the energy sector biomass burning is the major source of carbon dioxide emission contributing 81% followed by burning of petroleum products which contributed the remaining 19%.

3. The major agricultural activities which that generate carbon dioxide are bush burning and crop residue burning.

4. Comparing Ghana’s emissions with the rest of the world, the Environmental Protection Agency noted that two thirds of the total global carbon dioxide emission results from the burning of fossil fuels (coal, oil and gas) in electricity generation, industry, as heating and cooking fuel and in motor vehicles. The remaining one third of the global emission is due to deforestation. Most of the fossil fuel combustion occurs in the industrialised countries: United States of America and the former USSR each contributes one fifth of the world’s fuel burning carbon dioxide emissions followed by China, Japan, Germany, United Kingdom and Canada. Each American contributes nearly 100 times as much carbon dioxide as a Ghanaian. The industrialised countries who depend essentially on fossil fuels are therefore concerned with greening of the fossil fuels making them less harmful to the environment. We have an opportunity to create more greens thereby enhancing the capacity of the global carbon dioxide sink.

5. The global community shares one big sink: the atmosphere although we do not share the sources in the same way that we share the sink. And irrespective of the location of the carbon dioxide input the impacts affect all of us including the deprived and poor in the rural village.

6. The main issue facing us in Ghana is how to sustain and enhance the country’s forestry resources base not only as a source of food, fuel and shelter but also as a global sink for the world’s greenhouse gases.

7. Improving the efficiency of fuel burning and thermal conversion technologies is an equally important activity that would yield financial benefits in reduced petroleum imports as well as improved living conditions through reduced emission of greenhouse gases. The technologies will include thermal power plant combustion systems, high speed internal combustion engines for land and air transport as well domestic woodfuel burning technologies.

8. Simple wood fuel burning stoves are as important as the advanced fossil fuel burning technologies when we consider GHG emissions as well as monetary costs.

9. The major source of GHGs however is the slash and burn agricultural practice. Perhaps we should look at novel burning techniques: fuel cells may be?
LECTURE DELIVERED

- Introduction
- Fuels
- Basic principles and processes
- Engineering applications
- Emissions
- Summary and conclusions
Figure 1.1 Typical applications of combustion science

- Steam generation
- Heat transfer
- Space heating
- Turbojet propulsion
- Food processing
- Fire safety
- Waste incineration
- I.C. engine propulsion
- Welding
- Rocket propulsion
Chemical Equations—Conservation of Mass

- $12\text{kg C} + 32\text{kg O}_2 \rightarrow \text{CO}_2 \rightarrow 37790 \text{kJ/kg}$
- $\text{C} + \text{O} \rightarrow \text{CO}_2$
- Complete and incomplete combustion
- Combustion with air: volumetric 21% oxygen, 79% nitrogen; gravimetric 23.3% oxygen, 76.6% nitrogen includes inert gases such as argon. Excess air, stoichiometric air
- Predict analysis of products and determine stoichiometric air fuel ratio
- Experimental product analysis – Orsat apparatus
FIRST LAW OF THERMODYNAMICS

- Enthalpy of Combustion
- Adiabatic and Flame Temperatures
- Combustion Efficiency
- Power Plant Efficiency
- Dissociation

SECOND LAW AND CHEMICAL EQUILIBRIUM: GIBBS FUNCTIONS

- Equilibrium Composition
- Equation for Dissociation and Equilibrium Constant
Figure 2.7  Total mixtures energy lines vs. temperature

\[ n_c = \frac{\Delta H}{\Delta H_c} \]

H-T diagram and combustion efficiency

initial (reactant) state

\[ \Delta H_c \]

final (product) state

constant composition lines

reactants

incomplete combustion products

complete combustion products
Figure 3.8  Equilibrium constants vs. temperature for various reactions.
DETONATION AND DEFLAGRATION

- Deflagration is a combustion wave propagating at subsonic speed
- Detonation is a combustion wave propagating at supersonic speed
- A subsonic reaction front that passes through a reactive mixture, termed deflagration is also called a flame. They are either premixed or diffusion flames.
- Reactions within flames can be described using kinetics; they are determined by molecular collision frequencies and mean free paths.
- Thermal and radical generated e-m waves are produced by propagating reaction zones and result in visible or luminous flame emissions
- Stoichiometric and lean hydrocarbon flames appear blue in the kinetic zone while fuel rich flames are green. Flames with regions of high carbon particulate concentrations will appear yellow.
- Soot producing flames, having high concentration of carbon with thermally excited blackbody radiant heat transfer may be beneficial in some applications, such as firewood cooking stoves.
- Ignition temperature
- Flammability limits

Figure 5.1 Schematic of a premixed laminar flame above a Bunsen burner
Schematic diagram of a stationary one-dimensional combustion wave (detonation wave).
TABLE 1: Qualitative Differences Between Detonation and Deflagration in Gases

<table>
<thead>
<tr>
<th></th>
<th>Detonation</th>
<th>Deflagration</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\frac{U_d}{C_1}$</td>
<td>5-10</td>
<td>0.0001-0.03</td>
</tr>
<tr>
<td>$\frac{U_d}{U_1}$</td>
<td>0.4-0.7 (deceleration)</td>
<td>4-6 (acceleration)</td>
</tr>
<tr>
<td>$\frac{P_2}{P_1}$</td>
<td>13-55 (compression)</td>
<td>$\approx 0.98$ (slight expansion)</td>
</tr>
<tr>
<td>$\frac{T_2}{T_1}$</td>
<td>8-21 (heat addition)</td>
<td>4-16 (heat addition)</td>
</tr>
<tr>
<td>$\frac{P_2}{P_1}$</td>
<td>1.7-2.6</td>
<td>0.06-0.25</td>
</tr>
</tbody>
</table>

Data taken by Friedman

TABLE 2: Approximate Ignition Temperatures in 1-atm Air

<table>
<thead>
<tr>
<th>Combustible</th>
<th>Formula</th>
<th>°F</th>
<th>°C</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sulfur</td>
<td>S</td>
<td>470</td>
<td>245</td>
</tr>
<tr>
<td>Charcoal</td>
<td>C</td>
<td>650</td>
<td>345</td>
</tr>
<tr>
<td>Fixed carbon (bituminous coal)</td>
<td>C</td>
<td>765</td>
<td>405</td>
</tr>
<tr>
<td>Fixed carbon (semibituminous coal)</td>
<td>C</td>
<td>870</td>
<td>465</td>
</tr>
<tr>
<td>Fixed carbon (anthracite)</td>
<td>C</td>
<td>840-1115</td>
<td>450-600</td>
</tr>
<tr>
<td>Acetylene</td>
<td>C$_2$H$_2$</td>
<td>580-825</td>
<td>305-440</td>
</tr>
<tr>
<td>Ethane</td>
<td>C$_2$H$_4$</td>
<td>880-1165</td>
<td>470-630</td>
</tr>
<tr>
<td>Ethylene</td>
<td>C$_2$H$_6$</td>
<td>900-1020</td>
<td>480-550</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>H$_2$</td>
<td>1065-1095</td>
<td>575-590</td>
</tr>
<tr>
<td>Methane</td>
<td>CH$_4$</td>
<td>1170-1380</td>
<td>630-765</td>
</tr>
<tr>
<td>Carbon monoxide</td>
<td>CO</td>
<td>1130-1215</td>
<td>610-665</td>
</tr>
<tr>
<td>Kerosene</td>
<td>-</td>
<td>490-560</td>
<td>255-295</td>
</tr>
<tr>
<td>Gasoline</td>
<td>-</td>
<td>500-800</td>
<td>260-425</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Compound</th>
<th>Leanest</th>
<th>Richest</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acetone ($C_3H_6O$)</td>
<td>3.10</td>
<td>11.15</td>
</tr>
<tr>
<td>Acetylene ($C_2H_2$)</td>
<td>2.50</td>
<td>80.00</td>
</tr>
<tr>
<td>Ammonia ($NH_3$)</td>
<td>16.10</td>
<td>26.60</td>
</tr>
<tr>
<td>Benzene ($C_6H_6$)</td>
<td>1.41</td>
<td>7.10</td>
</tr>
<tr>
<td>Butane ($C_4H_{10}$)</td>
<td>1.86</td>
<td>8.41</td>
</tr>
<tr>
<td>Butyl ($C_4H_{16}$)</td>
<td>1.45</td>
<td>11.25</td>
</tr>
<tr>
<td>Butylene ($C_4H_8$)</td>
<td>1.98</td>
<td>9.65</td>
</tr>
<tr>
<td>Carbon Monoxide (CO)</td>
<td>12.50</td>
<td>74.20</td>
</tr>
<tr>
<td>Ethane ($C_2H_6$)</td>
<td>3.22</td>
<td>12.45</td>
</tr>
<tr>
<td>Ethyl ($C_2H_5O$)</td>
<td>4.25</td>
<td>18.95</td>
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<tr>
<td>Ethylene ($C_2H_4$)</td>
<td>3.05</td>
<td>28.60</td>
</tr>
<tr>
<td>Heptane ($C_7H_{16}$)</td>
<td>1.00</td>
<td>6.70</td>
</tr>
<tr>
<td>Hexane ($C_6H_{14}$)</td>
<td>1.27</td>
<td>6.90</td>
</tr>
<tr>
<td>Hydrogen ($H_2$)</td>
<td>4.00</td>
<td>74.20</td>
</tr>
<tr>
<td>Methane ($CH_4$)</td>
<td>5.00</td>
<td>14.00</td>
</tr>
<tr>
<td>Methyl ($CH_3O$)</td>
<td>7.10</td>
<td>36.50</td>
</tr>
<tr>
<td>Octane ($C_{10}H_{22}$)</td>
<td>0.95</td>
<td>-</td>
</tr>
<tr>
<td>Pentane ($C_5H_{12}$)</td>
<td>1.42</td>
<td>7.80</td>
</tr>
<tr>
<td>Propane ($C_3H_8$)</td>
<td>2.37</td>
<td>9.50</td>
</tr>
<tr>
<td>Propyl ($C_3H_{16}$)</td>
<td>2.15</td>
<td>13.50</td>
</tr>
<tr>
<td>Propylene ($C_3H_6$)</td>
<td>2.40</td>
<td>10.30</td>
</tr>
<tr>
<td>Propylene Oxide ($C_3H_6O$)</td>
<td>2.10</td>
<td>21.50</td>
</tr>
<tr>
<td>Toluene ($C_7H_8$)</td>
<td>1.45</td>
<td>6.75</td>
</tr>
</tbody>
</table>

Applications and Emissions

- Spray combustion systems
- Internal combustion engines
- Ghana study by EPA
Figure 1.2 The critical fuel–engine interface
Combustion Systems and Modelling

Fig. 1.3 Combustion driven heat engine family tree

- Continuous combustion
  - External
    - Brayton (gas turbine)
  - Internal
    - Non-condensing (Stirling)
    - Condensing (Rankine)

- Intermittent combustion
  - External
    - Diesel (rotary, reciprocal)
  - Internal
    - Otto (rotary, reciprocal)

- Homogeneous charge
- Stratified charge
- Direct injection
- Indirect injection
- Spark ignition
- Compression ignition
Four-stroke IC engine: (1) intake stroke; (2) compression stroke; (3) power stroke; and (4) exhaust stroke.
Figure 9.10  Typical IC engine performance map.
Spark-ignition constant-volume combustion characteristics
<table>
<thead>
<tr>
<th>Application</th>
<th>Configuration</th>
<th>Independent Variables</th>
<th>Structure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Prevaporizing system:</td>
<td></td>
<td>z</td>
<td>Steady nonburning</td>
</tr>
<tr>
<td>afterburners, lean combustors,</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>carburetors, ramjets</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Liquid-fueled rocket engines</td>
<td></td>
<td>z</td>
<td>Steady, more or less premixed</td>
</tr>
<tr>
<td>Gas-turbine combustors</td>
<td></td>
<td>z</td>
<td>Steady, diffusion flame</td>
</tr>
<tr>
<td>Industrial furnaces</td>
<td></td>
<td>x, y, z</td>
<td>Steady, diffusion flame</td>
</tr>
<tr>
<td>Diesel engines</td>
<td></td>
<td>t, x, y, z</td>
<td>Transient, diffusion flame,</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>ignition characteristics</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>needed</td>
</tr>
</tbody>
</table>

*After Faeth.\(^1\)
\(^1\)Simplest realistic approximation; all systems are axisymmetric or three-dimensional near the injector.
### Various Types of Injector Systems*

<table>
<thead>
<tr>
<th>Type</th>
<th>Configuration</th>
<th>Structure</th>
<th>Application</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Pressure-Atomizing Injectors</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Plain orifice</td>
<td>Hollow cone</td>
<td>Diesel engines</td>
<td></td>
</tr>
<tr>
<td>Pintle nozzle</td>
<td>Full cone or multiple cones</td>
<td>Diesel engines, gas turbines</td>
<td></td>
</tr>
<tr>
<td>Swirl nozzle (spill type return)</td>
<td>Hollow cone</td>
<td>Furnaces, gas turbines</td>
<td></td>
</tr>
<tr>
<td>Impinging jet</td>
<td>Fan spray</td>
<td>Rocket engines</td>
<td></td>
</tr>
<tr>
<td><strong>Twin-Fluid Injectors</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Internal Mixing</td>
<td>Full or hollow cone</td>
<td>Furnaces, gas turbines</td>
<td></td>
</tr>
<tr>
<td>External mixing</td>
<td>Hollow cone</td>
<td>Furnaces, gas turbines</td>
<td></td>
</tr>
</tbody>
</table>

*Combustion Systems and Modelling*
Internal Combustion Engine Gas Emissions

Carbon monoxide (CO):
CO, odourless, toxic gas (0.3% CO in air is lethal within 30 min), product of incomplete combustion.

Unburned Hydrocarbons (UHC):
C₅H₁₂, paraffins, olefins, and aromatics (odour and carcinogenic constituents), products of incomplete combustion

Partially Burned Hydrocarbons (PHC):
C₅H₁₀, CHO, aldehydes; C₅H₁₀, CO, Ketones; and C₅H₁₂, COOH, carboxylic acids; quenched products of low-temperature combustion.

Nitric oxides (NOₓ):
NO, nitric oxide, colourless and odourless gas; NO₂, nitrogen dioxide, reddish orange gas, corrosive and toxic; N₂O, nitrous oxide, colourless, odourless laughing gas. High-temperature by-products of lean combustion dissociation in excess air, major contributor to photochemical smog.

Sulphur Oxides (SOₓ):
SO₂, sulphur dioxide, non-flammable colourless gas, source of sulphuric acid (H₂SO₄) and acid rain, product of combustion of sulphur impurities in hydrocarbon fuels.
Figure 9.11 Typical gas chromatograph of exhaust gas emissions.
<table>
<thead>
<tr>
<th>Source and Type of Gas</th>
<th>CO₂</th>
<th>CH₄</th>
<th>N₂O</th>
<th>NOₓ</th>
<th>CO</th>
<th>CO₂ Equivalent</th>
<th>% Emission of CO₂ by Sectors</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>1. Energy Consumption</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A. Pet. Products</td>
<td>2537</td>
<td></td>
<td>0.30</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>B. Fuelwood</td>
<td>8059</td>
<td>35.2</td>
<td>0.24</td>
<td>5.7</td>
<td></td>
<td>307.7</td>
<td></td>
</tr>
<tr>
<td>C: Charcoal Cons.</td>
<td>1789</td>
<td>0.9</td>
<td>0.03</td>
<td>68.3</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>D: Charcoal Prod.</td>
<td>1104</td>
<td>25.3</td>
<td>0.8</td>
<td>42.1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Energy Subtotal</strong></td>
<td>13489</td>
<td>61.4</td>
<td>0.57</td>
<td>6.5</td>
<td>418.1</td>
<td>18766.3</td>
<td>15.6</td>
</tr>
<tr>
<td><strong>2. Industry</strong></td>
<td>1920</td>
<td></td>
<td>50</td>
<td>1920</td>
<td></td>
<td>1.6</td>
<td></td>
</tr>
<tr>
<td><strong>Subtotal</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>3. Agriculture</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A. Livestock</td>
<td></td>
<td>921</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>B. Rice Cultivation</td>
<td></td>
<td></td>
<td>16.5</td>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>C. Savannah Burning</td>
<td>7431</td>
<td>11.6</td>
<td>0.10</td>
<td>3.4</td>
<td></td>
<td>306</td>
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<td>D. Agricultural Res.</td>
<td>6859</td>
<td>13.3</td>
<td>0.40</td>
<td>8.2</td>
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<td>279</td>
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<tr>
<td><strong>Agricultural Subtotal</strong></td>
<td>14290</td>
<td>962.4</td>
<td>0.50</td>
<td>11.6</td>
<td>585</td>
<td>95236.69</td>
<td>7.9</td>
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<tr>
<td><strong>4. Waste</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A: Landfills</td>
<td>84</td>
<td>30.4</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>B: Wastewater - Industrial</td>
<td></td>
<td>11.2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>- Municipal</td>
<td></td>
<td>12.8</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>WASTE SUBTOTAL</strong></td>
<td>84</td>
<td>54.4</td>
<td></td>
<td></td>
<td></td>
<td>4653.6</td>
<td>3.8</td>
</tr>
<tr>
<td><strong>TOTAL EMISSIONS</strong></td>
<td>29783</td>
<td>1078.2</td>
<td>1.07</td>
<td>18.1</td>
<td>1053.1</td>
<td></td>
<td></td>
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<tr>
<td>Conversion Factors</td>
<td>1</td>
<td>84</td>
<td>210</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>CO₂ Equivalent</strong></td>
<td>29783</td>
<td>90,568.8</td>
<td>224.7</td>
<td></td>
<td>120,576.5</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Percentage Emission of CO₂ by type</strong></td>
<td>24.7</td>
<td>75.1</td>
<td>0.2</td>
<td></td>
<td></td>
<td>100</td>
<td></td>
</tr>
</tbody>
</table>

COMBUSTION MODELING AT THE UNIVERSITY OF SCIENCE AND TECHNOLOGY, KUMASI

Abeeku Brew-Hammond,
Senior Lecturer
Department of Mechanical Engineering
University of Science and Technology
Kumasi, Ghana

Outline

1. Simple Combustion Analysis
2. In-House Software
3. Off-the-Shelf Software
4. Challenges Ahead

Example 1: To Determine the Enthalpy of Combustion
\[ \Delta H_R = H_p - H_r \]

N.B.
\[ \Delta H_R : \text{Enthalpy of Combustion} \]
\[ \text{Enthalpy of Reaction} \]
\[ \text{Heat of Reaction (at constant pressure)} \]
Higher Heating Value (HHV): \( \Delta H_R, \text{H}_2\text{O} \text{ - Liquid} \)
Lower Heating Value (LHV)
\( \Delta H_R, \text{H}_2\text{O} \text{ - Gas} \)

Enthalpy of Formation, \( \Delta H_f = \Delta H_R \) for the formation of a substance from its elements in their most stable form.

\[
\text{CO} + \frac{1}{2}\text{O}_2 \rightarrow \text{CO}_2
\]

\[
\Delta H_{R, 1000K} = \frac{\Sigma N (h)_{1000K} - h_{\text{ref}} + \Delta h_{f,\text{ref}}}{\text{products}} - \frac{\Sigma N (h)_{1000K} - h_{\text{ref}} + \Delta h_{f,\text{ref}}}{\text{reactants}}
\]

**Rule Sheet**

\[ \text{delHR} = \text{SUMHr} - \text{SUMHp} \]

:Reactants and products at the same temperature

\[ \text{SUMHr} = \text{NCO} \times (h \text{CO} - h_{\text{refCO}} + h_{\text{fCO}}) + \text{NO2} \times (h \text{O2} - h_{\text{refO2}} + \theta) \]

\[ \text{SUMHp} = \text{NCO2} \times (h \text{CO}_2 - h_{\text{refCO2}} + h_{\text{fCO2}}) \]

Ideal gas properties for mixtures
call \( h (T', \text{O}_2; h \text{O2}) \)
call \( h (T', \text{CO}; h \text{CO}) \)
call \( h (T', \text{CO}_2; h \text{CO}_2) \)

**Variable Sheet**

<table>
<thead>
<tr>
<th>St</th>
<th>Input</th>
<th>Name</th>
<th>Output</th>
<th>Unit</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>L</td>
<td></td>
<td>delHR</td>
<td>-282600</td>
<td>kj/kmol</td>
<td>Enthalpy of reaction/kmol CO</td>
</tr>
<tr>
<td>L</td>
<td></td>
<td>SUMHr</td>
<td>-360100</td>
<td>kj/kmol</td>
<td>Absolute enthalpy of products/kmol CO</td>
</tr>
<tr>
<td>L</td>
<td></td>
<td>SUMHp</td>
<td>-77490</td>
<td>kj/kmol</td>
<td>Absolute enthalpy of reactants/kmol CO</td>
</tr>
<tr>
<td>L</td>
<td></td>
<td>NCO2</td>
<td>42760</td>
<td>kj/kmol</td>
<td>Number of moles CO2 per mole CO</td>
</tr>
<tr>
<td>9364</td>
<td></td>
<td>hCO2</td>
<td>42760</td>
<td>kj/kmol</td>
<td>Enthalpy (molar basis)</td>
</tr>
<tr>
<td>-393522</td>
<td>hrefCO2</td>
<td>42760</td>
<td>kj/kmol</td>
<td>hCO2 at 298.15 K</td>
<td></td>
</tr>
<tr>
<td>0.5</td>
<td></td>
<td>NO2</td>
<td>31380</td>
<td>kj/kmol</td>
<td>Number of moles O2 per mole CO</td>
</tr>
<tr>
<td>L</td>
<td></td>
<td>hO2</td>
<td>31380</td>
<td>kj/kmol</td>
<td>Enthalpy (molar basis)</td>
</tr>
<tr>
<td>1</td>
<td></td>
<td>NCO</td>
<td>30360</td>
<td>kj/kmol</td>
<td>Number of moles CO</td>
</tr>
<tr>
<td>8671</td>
<td></td>
<td>hCO</td>
<td>30360</td>
<td>kj/kmol</td>
<td>hCO at 298.15 K</td>
</tr>
<tr>
<td>-110530</td>
<td>hrefCO</td>
<td>30360</td>
<td>kj/kmol</td>
<td>hCO at 298.15 K</td>
<td></td>
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<tr>
<td>8683</td>
<td></td>
<td>hrefO2</td>
<td>30360</td>
<td>kj/kmol</td>
<td>hO2 at 298.15 K</td>
</tr>
<tr>
<td>L</td>
<td>1000</td>
<td>T</td>
<td></td>
<td>K</td>
<td>Temperature</td>
</tr>
</tbody>
</table>
CO + ½O₂ → CO₂

Example 2: To Determine Heat Transfer per kg of Fuel

\[ \text{CH}_4 + 2\text{O}_2 + 2(3.76)\text{N}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O} + 2(3.76)\text{N}_2 \]

\[ Q = h_f - h_L = \Sigma N (h_f - h_{ref} + \Delta h_{f,ref}) - \Sigma N (h_i - h_{ref} + \Delta h_{i,ref}) \]

products reactants

= ...................... (37.5 MJ/kg)
Tahedal Thermal Power Plant (Combined Cycle Gas Turbine)
Simple Gas Turbine System

Key Simulation Assumptions
1. A heat transfer process from an external source replaces the combustion process.
2. The working substance is treated as the air of fixed composition. The air is an ideal gas and has a constant specific heat.

**********INPUT VALUES**********

Mass of airflow into the compressor = 397.95Kg/sec
Mass of fuel-flow into combustion chamber = 8.33Kg/sec
Mass of water or steam injected for NOx control = 3.65Kg/sec
Ambient air temperature = 25°C

Cp of air at compressor inlet = 1.0025KJ/KgK
Cp of air at combustion chamber outlet = 1.1502KJ/KgK
Cp of steam at inlet of CC = 1.85KJ/KgK
Cp of steam at outlet of CC = 2.288KJ/KgK
Calorific Value of fuel = 43011 KJ/Kg
Compressor Discharge Pressure = 10.75

*****CALCULATED VALUES*****

Compressed air temperature = 322.1153°C
Temperature of combustion products = 987.8278°C
Exhaust gas temperature = 504.0322°C

The heat generated in the combustion chamber = 313,884.4137 KJ/sec
The work input into the compressor = 118,532.6444 KJ/sec
The turbine work output = 228110.328179145 KJ/sec
Power generated = 109,577.6838 KJ/s

The simple cycle efficiency, Netg1 = 0.2804
Combustion Systems and Modelling

Mass Flow Rate of Fuel, kg/s

Power Output, MW

Thermal Efficiency, %

Ambient Temperature

Petroleum Refinery Processes
FIG 1-1 PRINCIPAL FLOW DIAGRAM OF MATERIALS IN AN INTEGRATED PETROLEUM REFINERY FOR PRODUCING VARIOUS FUELS AND RAW MATERIALS FOR PETROCHEMICAL PLANTS
PHOENICS Software
(Recompilable Version - more flexible and user programmable)

Fees for academic use:

Annual licence: £1,900 or
Perpetual licence: £4,752 plus
Software Maintenance: £713 plus
Fortran compiler (each): £300

Fees for unlimited use

2.5 times the above.

CHALLENGES AHEAD

1. Consolidate and Expand utilisation of cheaper/simpler software packages by students (undergraduate and postgraduate)

2. Refine and further develop specialised application software (e.g. power plant simulation)

3. Seek assistance from other organisations/institutions to obtain more sophisticated software packages
INTRODUCTION TO TURBULENT COMBUSTION

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Grande Voie de Vigne F.
Chatenay Malabry Cedex
France

ABSTRACT

Combustion is a widely used technique in energy transformation and is encountered in many practical systems such as heaters, domestic and industrial furnaces, thermal power plants, automotive or aeronautical engines, rocket engines. In most applications, combustion occurs in turbulent gaseous flows. Combustion may be characterised by a strong and irreversible heat release taking place in very thin zones. The combustion reaction rate is also highly non-linear leading to modelling difficulties.

The scope of this first lecture is to briefly recall some fundamental aspects of combustion phenomena; premixed and non-premixed situations, laminar and turbulent flames, combustion instabilities and to emphasise the difficulties encountered in turbulent combustion understanding and modelling. These fundamental phenomena will be illustrated from description of simple laboratory experiments.

1. INTRODUCTION

1.1 Preliminary comments

Combustion is widely used in energy transformation and is encountered in many practical systems to produce heat (heaters, boilers, domestic or industrial furnaces), electricity (thermal power plants), in transports (automotive and aeronautical engines, rocket engines) or for waste destruction. Combustion may be defined as one (or several) irreversible chemical reaction(s) with high heat release between fuel and oxidizer, according to the global scheme:

\[ \text{Fuel} + \text{oxidizer} \rightarrow \text{Products} + \text{heat} \]

Combustion phenomena are characterized by:

- a strong and irreversible heat release. Heat release occurs in very thin zones (typical flame thicknesses \( \delta_L \) are about 0.1 to 1 mm) and induces strong temperature gradients (temperature ratio between burnt and unburnt gases, \( T_b/T_u \) are about 5 to 7) leading to strong heat transfers and large density variations.

- a stiff highly non linear chemical source (Arrhenius law reaction rate).
Various gaseous, liquid or solid fuels may be used. Most popular fuels are wood, coal, hydrocarbons (methane $\text{CH}_4$, propane $\text{C}_3\text{H}_8$, gasoline, kerosene, fuel,...), hydrogen ($\text{H}_2$),.... Oxidizer is generally oxygen contained in air but, in some systems, pure oxygen may be used (rocket engines, some industrial furnaces) because of higher burnt gases temperatures and no inert nitrogen storage but induces safety problems. In some very specific applications, other oxidizers may be used (pyrotechnic rocket engines).

Various coupling mechanisms occur in turbulent flames. **Chemical reaction schemes** must be known to estimate the consumption rate of fuel, the formation of combustion products and pollutant species and are required to predict ignition, stabilization or extinction. **Mass transfers** of chemical species by molecular diffusion, convection and turbulent transport are also an important ingredient of combustion processes. The heat release due to chemical reactions induces strong conductive, convective or radiative **heat transfers** inside the flow field and with the surroundings (walls for example). This thermal energy is then used for heating or is converted into mechanical energy in a gas turbine or in a piston engine. Of course, gaseous combustion requires the description of the flow field (**fluid mechanics**). In some systems, other aspects may be also involved. Two (liquid fuel) and three (solid fuel) phase systems may be encountered. Phenomena such as spray formation and vaporization, droplet combustion,... have to be taken into account. Soot formation leads to carbon particles which will be transported by the flow motions, and generate radiative heat transfer.

The main difficulty in turbulent combustion modeling comes from the interaction between turbulence and heat release. A large range of time and length scales is encountered: turbulent scales such as turbulent kinetic energy $k$, integral, $l$, and Kolmogorov, $l_k$, length scales, ... and chemical scales (flame thickness, chemical time scales ...). For example, in most practical situations, the fuel oxidation reaction occurs in short times compared to turbulence times but other reactions such as pollutant formations have longer characteristic times.

The aim of this lecture is to propose an introduction to turbulent combustion phenomena and modeling.

Following a short presentation of the balance equations in reactive flows (§2), a first part is devoted to a brief description of laminar flames and how turbulent motions may affect combustion (§3). After a short presentation of the unsuccessful Taylor's expansion of the mean reaction rate (§4), physical analysis leading to turbulent combustion diagrams are developed (§5). Modeling tools available to derive turbulent combustion models are then described and the relations between a priori quite different formalisms are evidenced (§6). The three following sections are devoted to the various approaches developed to describe mean flow fields (Reynolds Averaged Navier-Stokes, or RANS): mean reaction rate (§7) and turbulent transport (§8) modeling in premixed turbulent combustion and reaction rate modeling in turbulent non-premixed situations (§9). A synthetic presentation have been chosen to exhibit the connections, in fact stronger than generally perceived, between the various approaches. In a last part, large eddy simulations (LES) is briefly discussed (§10). LES is today just starting to be applied to
combustion, but has been extensively used to describe non reacting flows and appears as a very promising tool, especially to predict combustion instabilities.

1.2 Practical importance of turbulent combustion

In most practical applications, combustion occurs in turbulent flows, where mass and heat transfers are higher and more efficient than in laminar flows. Accordingly, combustion in turbulent flows, or turbulent combustion has been extensively studied to understand the complex phenomena occurring in such situations and to develop relevant models. The final objective is to perform numerical simulations of practical systems to decrease development costs. Various criteria, depending on the final use of the system, may be involved: power optimization, reduced pollutant emissions... Up to now, some trends are well predicted by numerical simulations, but relevant simulations of an actual practical system are still far from being available. Let us also point out that pollutant emissions involve minor species (from few ppm to several percents) that have to be accurately predicted. To reduce pollutant emissions (unburnt hydrocarbons HC, carbon monoxide CO, ...) also generally corresponds to a more efficient combustion.

Two limiting cases depending on the introduction of reactants in the combustion zone are identified: perfectly premixed combustion and non premixed flames.

- (a) Perfectly premixed reactants

![Diagram of perfectly premixed reactants]

- (b) Non premixed reactants

![Diagram of non premixed reactants]

**Fig. 1 Premixed flame (a) and Non-premixed flame (b)**

- **Premixed combustion.** Reactants, fuel and oxidizer are perfectly mixed at the molecular level before entering the reaction zone (Fig. 1a). This situation is favorable in terms of burning efficiency (reactants are already mixed) but a flame is able to propagate in premixed reactants upstream of the burner, leading to safety problems.

- In non premixed combustion, the reactants are introduced separately in the reaction zone. The simplest geometry of a non premixed (or diffusion) flame is a mixing layer (Fig. 1b) or a fuel jet discharging in ambient air. In these situations, the flame is unable to propagate upstream but the reaction rate may be limited by the mixing of the reactants, controlled by convection,
molecular diffusion and turbulent transport. Non-premixed flames are also easier to build than premixed flames because no well-controlled burning mixtures have to be prepared.

In practical systems, combustion occurs in gaseous flows. Accordingly, a second classification has to be considered depending on the flow type, laminar or turbulent. Four limiting regimes are then identified depending on the flow regimes (laminar or turbulent) and on the reactants introduction (premixed/non-premixed). On Fig. 2 these four situations are summarized with corresponding practical systems. Laminar combustion is found in a reduced number of applications (candle, lighter, Bunsen burner...). In fact, most practical systems involve turbulent combustion but laminar flames are important ingredients to describe and model practical systems and in a first step, main properties of laminar premixed and non premixed flames will be recalled (§ 3).

Figure 2: Classification of reacting flows depending on the introduction of reactants (premixed or not) and on the flow characteristics (laminar or turbulent) corresponding to practical systems are also indicated.
2 Balance equations

2.1 Instantaneous balance equations

The basic set of balance equations comprises the classical Navier-Stokes, species and energy transport equations. These instantaneous local balance equations (Barrère and Prud'homme 1973; Williams 1985; Kuo 1986) are, using the classical lettering:

- **Mass**:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0
\]  

(2.1)

- **Momentum** (i = 1, 2, 3):

\[
\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + F_i
\]  

(2.2)

where \( \tau_{ij} \) denote viscous force tensor and \( F_i \) a volume force.

- **Species** (N species with \( k = 1, \ldots, N \)):

\[
\frac{\partial \rho Y_k}{\partial t} + \frac{\partial \rho u_j Y_k}{\partial x_j} = -\frac{\partial J^k_j}{\partial x_j} + \dot{\omega}_k
\]  

(2.3)

where \( J^k_j \) is the molecular diffusion flux of species \( k \) and \( \dot{\omega}_k \) the mass production rate of species \( k \) per unit volume.

- **Total enthalpy** \( h = h + u_i u_i/2 \):

\[
\frac{\partial \rho h}{\partial t} + \frac{\partial \rho u_j h}{\partial x_j} = \frac{\partial p}{\partial t} + \frac{\partial}{\partial x_j} \left( J^h_j + u_j \tau_{ij} \right) + u_j F_j
\]  

(2.4)

where \( u_j \tau_{ij} \) and \( u_j F_j \) denote respectively the power due to viscous and volume forces.

These equations are closed by expressions for the species molecular fluxes and the viscous forces. In practical situations, all fluids are assumed to be Newtonian, i.e. the viscous tensor is given according to the Newton law:

\[
\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \delta_{ij} \frac{\partial u_k}{\partial x_k}
\]  

(2.5)

where the laminar viscosity, depending on the fluid properties is introduced. \( \delta_{ij} \) is the Kronecker symbol.

Species molecular diffusivities are generally described using the Fick law, assuming a major species, leading to:

\[
J^k_j = \frac{\mu_k}{S_c k} \frac{\partial Y_k}{\partial x_j}
\]  

(2.6)
where $S_{ck}$ is the Schmidt number of the species $k$, defined as:

$$S_{ck} = \frac{\mu_k}{\rho D_k}$$  \hspace{1cm} (2.7)

where $D_k$ is the molecular diffusivity of species $k$ relatively to the major species.

More complex expressions may be used to describe multi-species molecular diffusion. Soret effect (species diffusion under temperature gradients) and molecular transport due to pressure gradients are neglected here.

Enthalpy diffusion is described according to the Fourier law:

$$J_i^h = -\frac{\mu_i}{Pr} \left[ \frac{\partial h}{\partial x_i} + \sum_{k=1}^{N} \left( \frac{Pr}{Sc_k} - 1 \right) k_k \frac{\partial Y_k}{\partial x_i} \right]$$  \hspace{1cm} (2.8)

where $Pr$ is the Prandtl number, comparing the diffusive transport of momentum (viscous forces) and enthalpy. In the previous expressions, radiative heat transfer and Dufour effect (enthalpy diffusion under mass fraction gradients) are neglected. The Prandtl number is written as a function of the thermal diffusivity $\lambda$ and the constant pressure specific heat $C_p$:

$$Pr = \left( \frac{\mu C_p}{\lambda} \right)$$  \hspace{1cm} (2.9)

Then, the Lewis number $Le_k$ of species $k$, comparing thermal and mass diffusivity is introduced:

$$Le_k = \left( \frac{Sc_k}{Pr} \right) = \left( \frac{\lambda}{\rho C_p D_k} \right)$$  \hspace{1cm} (2.10)

Under the assumption of unity Lewis number, the enthalpy diffusive flux (Eq. 2.8) becomes simpler and mass fraction and enthalpy balance equations becomes formally identical. This assumption is generally made to simplify turbulent flame modeling. Nevertheless, thermo-diffusive instabilities occur when the Lewis number is lower than unity (for example for hydrogen). These instabilities increase the flame area and, accordingly, the global reaction rate (Williams 1985; Trouvé and Poinset 1994).

2.2 Reynolds and Favre averaging

Unfortunately, instantaneous balance equations can be numerically solved only in some very simple cases (direct numerical simulations, Poinset 1996). This limitation is due to the large of time and length scales present in the flow that have to be described. An additive step is introduced by averaging the balance equations to describe only the mean flow field (turbulence structures effects are modeled and these structures have no longer to be described in the simulation). Each quantity $Q$ is split into a mean $\overline{Q}$ and a deviation from the mean noted $Q'$:

$$Q = \overline{Q} + Q' \quad \text{with} \quad \overline{Q'} = 0$$  \hspace{1cm} (2.11)
Then, the previous instantaneous balance equations may be ensemble averaged to derive transport equations for the mean quantity $\bar{Q}$. This classical Reynolds averaging technique, widely used in non-reacting fluid mechanics, leads to unclosed quantities such as $\rho'\bar{Q}'$ that are unknown and must be modeled.

In turbulent flames, density fluctuations are observed because of the thermal heat release, and Reynolds averaging induces some difficulties. Averaging the mass balance equation leads to:

$$\frac{\partial \bar{p}}{\partial t} + \frac{\partial}{\partial x_i} \left( \bar{p} \bar{u}_i + \rho' \bar{u}_i' \right) = 0$$

(2.12)

where velocity and density fluctuations correlations $\rho' u_i'$ needs to be described. To avoid the explicit modeling of such correlations, a Favre (mass weighted) average $\bar{Q}$ is introduced and any quantity is then splitted as $Q = \bar{Q} + Q'$:

$$\bar{Q} = \frac{\rho \bar{Q}}{\bar{p}} ; \quad \bar{Q}' = \frac{\rho (Q - \bar{Q})}{\bar{p}} = 0$$

(2.13)

Then, the Favre averaged continuity equation:

$$\frac{\partial \bar{p}}{\partial t} + \frac{\partial \bar{p} \bar{u}_i}{\partial x_i} = 0$$

(2.14)

is formally identical to the Reynolds averaged continuity equation for constant density flows. This result is true for any balance equations (momentum, energy, mass fractions...). Nevertheless, Favre averaging is only a mathematical formalism leading to the following comments:

- There is no simple relation between Favre, $\bar{Q}$, and Reynolds, $\bar{Q}$, averages. A relation between $\bar{Q}$ and $\bar{Q}$ requires the knowledge of density fluctuations correlations $\rho'\bar{Q}'$ remaining hidden in Favre averaged quantities (see § 7.3.3):

$$\bar{\rho} \bar{Q} = \bar{\rho} \bar{Q} + \bar{\rho} \bar{Q}'$$

(2.15)

- Comparisons between numerical simulations, providing Favre averaged quantities $\bar{Q}$ with experimental results are not obvious. Most experimental techniques determine Reynolds averaged data $\bar{Q}$ and differences between $\bar{Q}$ and $\bar{Q}$ may be significant (§ 7.3.3 and Fig. 15).

- Some authors (Hussain 1983; Liu 1988) have proposed to split each quantity $Q$ into mean, coherent and fluctuating parts:

$$Q = \bar{Q} + Q_c + Q'$$

(2.16)

to distinguish between mean flow contribution, coherent structure effects and uncoherent turbulent motions. This approach is attractive, but leads to a larger number of unclosed
Species ($\overline{u_j^nY_k^n}$) and temperature ($\overline{u_j^nT_k^n}$) turbulent fluxes. These fluxes are generally closed using a "classical" gradient expression:

$$\overline{\mu_t u_j^n Y_k^n} = -\frac{\mu_t}{S_c k_t} \frac{\partial \tilde{Y}_k}{\partial x_j}$$  \hspace{1cm} (2.21)

where $\mu_t$ is the turbulent viscosity, estimated from the turbulence model, and $S_c k_t$ a turbulent Schmidt number for species $k$.

Nevertheless, some theoretical and experimental works (Bray et al. 1981; Shepherd et al. 1982) have evidenced that this assumption may be clearly wrong in some premixed turbulent flames and counter-gradient turbulent transport (i.e. in an opposite direction compared to the one predicted from Eq. (2.21)) may be observed (see § 7.3.4 and § 8).

Laminar diffusive fluxes $\overline{J_k^F}, \overline{J_j^F}$... are always neglected against turbulent transport, assuming a sufficiently large turbulence level (large Reynolds numbers limit).

Species chemical reaction rates $\overline{\omega_k}$. Turbulent combustion modeling is generally focused on the closure of these mean reaction rates.

Of course, these equations, coupled to ad-hoc models, allow only the determination of mean quantities that may be quite different from instantaneous ones...
3 Major properties of premixed, non-premixed and partially premixed flames

3.1 Laminar premixed flames

3.1.1 General properties

The structure of a laminar premixed flame is displayed in Fig. (3). Fresh gases (fuel and oxidizer) and burnt gases (combustion products) are separated by a thin reaction zone (typical flame thickness, $\delta_f$ are about 0.1 to 1 mm). A strong temperature gradient is observed (typical ratios between burnt and fresh gases temperatures are about 5 to 7). The main characteristic of a premixed flame is its ability to propagate towards the fresh gases. Because of the temperature gradient and the corresponding thermal fluxes, fresh gases are preheated and then start to burn. The local imbalance between diffusion of heat and chemical consumption leads to propagation of the front. The propagation speed $S_L$ of a laminar flame depends on various parameters (fuel and oxidizer compositions, fresh gases temperature, ... ) and is about 0.1 to 1 m/s. There is an interesting relation between the thermal flame thickness, $\delta_f$, the laminar flame speed, $S_L$ and the kinematic viscosity of the fresh gases, $\nu$:

$$Re_f = \frac{\delta_f S_L}{\nu} \approx 4.$$ (3.1)

The flame Reynolds number, $Re_f$, is then constant. This relation, derived, for example, from the Zeldovich / Frank-Kamenetskii (ZFK) theory (Williams 1955; Kuo 1986) is often implicitly used in theoretical derivation of turbulent premixed combustion models.

For a one-step irreversible simple chemical scheme:

$$Reactants \rightarrow Products$$

the chemical reaction is usually described using a progress variable $c$ such as $c = 0$ in the fresh gases and $c = 1$ in the fully burnt ones. This progress variable may be defined as a reduced temperature or a reduced mass fraction:

$$c = \frac{T - T_u}{T_b - T_u} \quad \text{or} \quad c = \frac{Y_F - Y_G}{Y_F^b - Y_G^b} \quad \text{(3.2)}$$

where $T$, $T_u$ and $T_b$ are respectively the local, the unburnt gases and the burnt gases temperatures. $Y_F$, $Y_F^b$ and $Y_G^b$ are respectively the local, unburnt gases and burnt gases fuel mass fractions. $Y_G^b$ is non-zero for a rich combustion (fuel in excess). For an unity Lewis number (same molecular and thermal diffusivities), without heat losses (adiabatic combustion) and compressibility effects, the two definitions (3.2) are equivalent and mass and energy balance equations reduce to a single balance equation for the $c$ progress variable:

$$\frac{\partial \rho c}{\partial t} + \nabla \cdot (\rho u c) = \nabla \cdot (\rho D \nabla c) + \dot{\omega} \quad \text{(3.3)}$$
3.2 Laminar diffusion flames

3.2.1 Introduction

In a nonpremixed (or diffusion) flame, fuel and oxidizer are initially separated. In the simplified view presented in Fig. 4, fuel and oxidizer are on both sides of a reaction zone where the heat is released. The reaction rate is essentially controlled by the molecular diffusion governing the feeding of the reaction zone with the reactants. Through diffusion of products towards both fuel and oxidizer sides, the thickness of the reactive and diffusive layer of Fig. 4 increases with time, and there is no steady solution. From this simple observation, in opposition with premixed flames:

- Diffusion flames do not exhibit a self-induced propagation mechanism, but are mainly mixing controlled.
- The thickness of a diffusion flame is not constant and depends on the local flow properties.

To understand very basic properties of diffusion flames, let us consider the irreversible single step chemical reaction between fuel and oxidizer:

\[ F + sO \rightarrow (1+s)P \]
Figure 4: Generic structure of a laminar diffusion flame.

where $s$ is the mass stoichiometric coefficient. In term of mass fraction, this chemical reaction may be written:

$$\nu_F Y_F + \nu_O Y_O \rightarrow \nu_P Y_P$$

where $Y_F$, $Y_O$ and $Y_P$ are the mass fraction of the fuel, the oxidizer and the product respectively. $\nu_i$ are the stoichiometric molar coefficients of the reaction, $W_i$ denote the species molar weight and $\dot{\omega}$ (mol.m$^{-3}$.s$^{-1}$) is the reaction rate. The balance equations for mass fractions and temperature are:

$$\rho \frac{\partial Y_F}{\partial t} = -\rho u \cdot \nabla Y_F + \nabla \cdot (\rho D_F \nabla Y_F) - \nu_F W_F \dot{\omega}$$

$$\rho \frac{\partial Y_O}{\partial t} = -\rho u \cdot \nabla Y_O + \nabla \cdot (\rho D_O \nabla Y_O) - \nu_O W_O \dot{\omega}$$

$$\rho \frac{\partial T}{\partial t} = -\rho u \cdot \nabla T + \nabla \left( \frac{\lambda}{c_p} \nabla T \right) + \frac{Q}{c_p} \dot{\omega}$$

Here the molecular diffusion is expressed using the Fick law, the chemical rate of fuel and oxidizer are respectively $\dot{\omega}_F = \nu_F W_F \dot{\omega}$ and $\dot{\omega}_O = \nu_O W_O \dot{\omega}$. $Q$ is the amount of heat released by the combustion of an unit mass of fuel.

The structure of diffusion flames may be represented in term of mixing between fuel and oxidizer. A mixture fraction $Z$ evolving from zero (oxidizer) to unity (fuel) through the diffusive-
layer is introduced:

\[
Z = \frac{\phi Y_F - Y_{O,\phi} + 1}{\phi + 1}
\]  

(3.4)

where \( Y_{F,\phi} \) is the fuel mass fraction in the fuel feeding stream (this mass fraction is lower than unity when the fuel is diluted). Similarly, \( Y_{O,\phi} \) is the oxidizer mass fraction in the oxidizer stream (for instance, in air, \( Y_{O,\phi} \approx 0.23 \)). \( \phi \) is the equivalence ratio of the reaction:

\[
\phi = \frac{s Y_{F,\phi}}{Y_{O,\phi}}
\]  

(3.5)

with \( s = (\nu_0 W_O/\nu_F W_K) \). In addition, assuming that fuel and oxidizer molecular diffusivities are equal (i.e. \( D_F = D_O = D \)), \( Z \) is a conserved scalar, called a Schwab-Zeldovich variable, and follows the balance equation without source term:

\[
\frac{\partial \rho Z}{\partial t} + \frac{\partial \rho u_i Z}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \rho D \frac{\partial Z}{\partial x_i} \right)
\]  

(3.6)

\( Z \) features the following interesting properties:

- \( Z = 1 \) in the fuel stream.
- \( Z = 0 \) in the oxidizer stream.
- \( Z(z, t) \) measures the degree of mixing between fuel and oxidizer independently of the reactive activity.
- Under the hypothesis of infinitely fast chemistry (when fuel and oxidizer cannot coexist at the same location), the flame front is defined by the relation \( Y_F = Y_O = 0 \) and corresponds to the iso-surface \( Z = Z_{st} = 1/(\phi + 1) \).

### 3.2.2 Flame structure as a function of \( Z \)

Mass fractions and temperature balance equations may be reorganized into a new frame where \( Z \) is one of the coordinates (see for instance Williams 1985). When the gradients in the normal direction to the iso-\( Z_{st} \) dominate (i.e. weak curvature of the flame), the balance equation for the mass fractions becomes:

\[
\rho \frac{\partial Y_i}{\partial t} = \rho \chi \frac{\partial^2 Y_i}{\partial Z^2} + \dot{\omega}_i
\]  

(3.7)

where \( \chi \) is the scalar dissipation rate of the mixture fraction \( Z \):

\[
\chi = D \left( \frac{\partial Z}{\partial x_i} \frac{\partial Z}{\partial x_i} \right) = D |\nabla Z|^2
\]  

(3.8)
corresponding to the inverse of a time\textsuperscript{1}. As this time decreases, mass and heat transfers through the stoichiometric surface are enhanced.

Looking for a steady solution of Eq. (3.7), two limiting cases are identified (Fig. 5):

- **When no reaction occurs**, pure mixing between fuel and oxidizer develops, $\dot{w}_i = 0$:
  \begin{align*}
  Y_F(Z) &= Y_{F,0} Z \\
  Y_O(Z) &= Y_{O,0} (1 - Z) \\
  T(Z) &= (T_{F,0} - T_{O,0}) Z + T_{O,0}
  \end{align*}

- **When the chemistry is infinitely fast**, fuel and oxidizer cannot co-exist. Then, $Y_F Y_O = 0$ elsewhere, corresponding to $Y_F = 0$ on the air side of the flame ($Z < Z_{fl}$) and $Y_O = 0$ ($Z > Z_{fl}$) on the fuel side.

\textsuperscript{1}Various definitions of the scalar dissipation $\gamma$ may be encountered depending on the authors. The density $\rho$ and a factor 2 may be introduced in definition (3.8).
Figure 5: Inner structure of non-premixed flames. The distribution in mixture fraction space of fuel, oxidizer and temperature lies between the infinitely fast chemistry limit and the pure mixing case. The thickness of the diffusive zone \( l_d \) is estimated from the scalar dissipation rate \( \chi \) at the stoichiometric surface, whereas the characteristic thickness of the reactive zone \( l_r \) depends on both \( l_d \) and the Damköhler number.
3.3 Experimental results: influence of turbulence on combustion

3.3.1 One-dimensional turbulent premixed flame

A statistically one-dimensional premixed flame propagating in a turbulent flow field is considered (fig. 6). In this situation, a planar flame, with a thickness $\delta_T$ and a propagation speed $S_T$ is observed. Generally, experimental results show that $S_T \gg S_L$ and $\delta_T \gg \delta_L$ where $S_L$ and $\delta_L$ are the corresponding premixed laminar flame speed and thickness respectively. Flame propagation measurements lead to empirical relations such as: (Abdel-Gayed et al. 1984; Abdel-Gayed and Bradley 1989):

$$\frac{S_T}{S_L} = 1 + \alpha \left( \frac{u'}{S_L} \right)^n$$

(3.9)

where $\alpha$ and $n$ are model constants of the order of unity, and $u'$ is the rms of the velocity fluctuations (or the square root of the turbulent kinetic energy $k$).

This expression, which only gives an order of magnitude because $S_T$ is not a well-defined quantity and depends strongly on the experimental configuration, clearly shows that the combustion is enhanced by turbulent motions. For large values of the velocity fluctuations, assuming $n = 1$, the turbulent flame speed $S_T$ becomes roughly independent on the laminar flame speed $S_L$ ($S_T \approx u'$).

Turbulence has two main effects:

- An increase of the flame area wrinkled by turbulence motions.
An increase of mass and heat transfers.

Damköhler (1940) links the turbulent flame speed \( S_T \) to the wrinkling of the flame surface and proposes the following relation:

\[
\frac{S_T}{S_L} = \frac{A_T}{A_L}
\]  

(3.10)

where \( A_L \) and \( A_T \) are the flame surface corresponding to the laminar and the turbulent flames respectively.

The ratio \( A_T/A_L \) is the flame wrinkling factor and may be estimated from the inverse of the turbulence integral length scale \( l_t \), which is proportional to the turbulent viscosity \( \nu_T \) and, accordingly to the Reynolds number \( Re \). Then, \( S_T/S_L \propto Re \). But this simple theory, in agreement with expression (3.9), is not valid for large Reynolds numbers where other effects may be encountered such as the so-called bending effect (for large Reynolds numbers, the turbulent flame speed is found to decrease when \( Re \) increases before the occurrence of a flame quenching).

### 3.3.2 Turbulent jet flame

In this configuration (Fig. 7), a jet of fuel is injected in ambient air. The flame length \( L_f \) may be experimentally estimated and the results qualitatively displayed in Fig. 8 as a function of the Reynolds number \( Re \):

\[
Re = \frac{u_0 d_0}{\nu}
\]

where \( u_0 \), \( d_0 \) and \( \nu \) are respectively the initial velocity, the diameter and the kinematic viscosity of the fuel jet stream.

The flame length \( L_f \) is found to linearly increase with the fuel flow rate or the Reynolds number \( Re \). For a sufficiently high Reynolds number, the flow becomes turbulent and the flame length \( L_f \) decreases before reaching a constant value independent on the Reynolds number \( Re \). The transition between laminar and turbulent region of the flame becomes closer and closer.
Figure 8: length $L_f$ of a jet flame as a function of the Reynolds number $Re = (u_0d_0/\nu)$.

of the injector lip. For sufficiently high injection velocities, the flame is lifted from the burner ("lifted flame") and then may be extinguished by "blow-off".

As the flame length $L_f$ remains constant when the Reynolds number (or the injection velocity) increases, the reaction rate is increased by turbulence and the combustion becomes more efficient.
4 A first simplified analysis: Taylor’s expansion

A direct approach to describe turbulent combustion is first discussed in this section. This simple formalism, based on series expansion, illustrates the difficulties arising from the non-linear character of chemical sources.

Consider a simple irreversible reaction between fuel (F) and oxidizer (O):

\[ F + s O \rightarrow (1 + s) P \]

where the fuel mass reaction rate \( \dot{\omega}_F \) is expressed from the Arrhenius law as:

\[ \dot{\omega}_F = -A \rho^2 T^b \bar{Y}_F \bar{Y}_O \exp \left( -\frac{E}{RT} \right) \]

(4.1)

A is the pre-exponential constant, \( E \) the activation energy and \( R \) the perfect gases constant.

As the reaction rate is highly non-linear, the averaged reaction rate \( \overline{\dot{\omega}_F} \) cannot be easily expressed as a function of the mean mass fractions \( \overline{\bar{Y}_F} \) and \( \overline{\bar{Y}_O} \), the mean density \( \bar{\rho} \) and the mean temperature \( \bar{T} \). The first simple idea is to expand the mean reaction rate \( \overline{\dot{\omega}_F} \) as a Taylor serie:

\[ e^{-(T_a/T)} = e^{-(T_a/\bar{T})} \left( 1 + \sum_{n=1}^{+\infty} P_n \frac{T_a^n}{\bar{T}^n} \right) \quad ; \quad T^b = \bar{T}^b \left( 1 + \sum_{n=2}^{+\infty} Q_n \frac{T_a^n}{\bar{T}^n} \right) \]

(4.2)

where \( P_n \) and \( Q_n \) are given by:

\[ P_n = \sum_{k=1}^{n} \frac{(-1)^{n-k}}{(n-k)!([k-1])^2 k} \frac{(T_a)^k}{\bar{T}} \]

\[ Q_n = \frac{b(b+1)...(b+n-1)}{n!} \]

(4.3)

The mean reaction rate, \( \overline{\dot{\omega}_F} \) becomes (Borghi 1978):

\[ \overline{\dot{\omega}_F} = -A \rho^2 T^b \bar{Y}_F \bar{Y}_O \exp \left( -\frac{E}{RT} \right) \left[ 1 + \frac{Y_F Y_O}{\bar{Y}_F \bar{Y}_O} + (P_1 + Q_1) \left( \frac{Y_F Y_O}{\bar{Y}_F \bar{Y}_O} \right) + \frac{Y_F Y_O}{\bar{Y}_F \bar{Y}_O} \right] \]

(4.4)

\[ + (P_2 + Q_2 + P_3 Q_3) \left( \frac{Y_F Y_O}{\bar{Y}_F \bar{Y}_O} \right) + \ldots \]

Equation (4.4) leads to various difficulties. First, new quantities such as \( Y_F Y_O \) have to be closed, using algebraic expressions or transport equations. Because of non-linearities, large truncature errors are also introduced when only few terms of the series expansion are taken into account. Expression (4.4) is quite complicated but is only valid for a simple irreversible reaction and cannot be easily extended to realistic chemical schemes (at least 9 species and 19 reactions for hydrogen combustion, several hundred species and several thousand reactions for hydrocarbon combustion). For these reasons, reaction rate closures in turbulent combustion are not based on (4.4) but are derived from physical analysis as described in the next section.
Nevertheless, this approach is used in some practical simulations where chemical times cannot be neglected against mechanical times for example in supersonic reacting flow fields (Villasenor et al. 1991) or to describe reaction in atmospheric boundary layer where the temperature $T$ may be roughly assumed to be constant (Nieuwstadt and Meeder 1997). In these situations, only the first two terms in the series expansion are kept. A segregation factor, $\alpha_{FO}$, is then introduced:

$$\alpha_{FO} = -\frac{\overline{Y_F Y_O'}}{\overline{Y_F Y_O}'} = \left(1 - \frac{\overline{Y_F Y_O'}}{\overline{Y_F Y_O}}\right)$$  \hspace{1cm} (4.5)

to characterize the mixing between the reactants $F$ and $O$. If they are perfectly separated ($\overline{Y_F Y_O} = 0$), $\alpha_{FO} = -1$. On the other hand, a perfect mixing ($\overline{Y_F Y_O'} = 0$) leads to $\alpha_{FO} = 0$. This segregation factor may be either postulated or provided by a balance equation (see Meeder and Nieuwstadt 1997 in the large eddy simulation context). Then, the mean reaction rate becomes:

$$\overline{\dot{w}_F} = -A (1 - \alpha_{FO}) \overline{\rho^2 T^b Y_F Y_O e^{-\frac{T}{T}}} \hspace{1cm} (4.6)$$
5 Physical analysis - Turbulent combustion diagrams

5.1 Introduction

As the mean reaction rate $\overline{\nu}k$ cannot be found from an averaging of Arrhenius laws, a physical approach is required to derive models for turbulent combustion. Turbulent combustion involves various lengths, velocity and time scales describing turbulent flow field and chemical reactions and the physical analysis is mainly based on comparison of these scales.

The first step in turbulent combustion is to ensure a turbulent flow field, characterized by the Reynolds number comparing turbulent transport to viscous forces:

$$Re = \frac{u'l_t}{v}$$  \hspace{1cm} (5.1)

where $u'$ is the velocity rms (related to the square root of the turbulent kinetic energy $k$), $l_t$ is the turbulence integral length scale and $v$ the kinematic viscosity of the flow.

Damköhler number compares the turbulent ($t_t$) and the chemical ($t_c$) time scales:

$$Da = \frac{t_t}{t_c}$$  \hspace{1cm} (5.2)

In the limit of high Damköhler numbers ($Da \gg 1$), the chemical time is short compared to the turbulent time, corresponding to a thin reaction zone distorted and convected by the flow field. The internal structure of the flame is not affected by turbulence and may be described as a laminar flame element called "flamelet". The turbulent structures wrinkle and strain the flame surface. On the other hand, a low Damköhler ($Da \ll 1$) corresponds to a slow chemical reaction. Reactants and products are mixed by turbulent structures before reaction. In this perfectly stirred reactor limit, the mean reaction rate may be expressed from Arrhenius laws using mean mass fractions and temperature, corresponding to the first term of the Taylor's expansion (4.4). Most practical situations correspond to high or medium values of the Damköhler numbers. It is worth noting that various chemical time scales may be encountered: fuel oxidation generally corresponds to short chemical time scales ($Da \gg 1$) whereas pollutant production or destruction such as CO oxidation or NO formation are slower ($Da \approx 1$).

In the following, only diagrams for turbulent combustion will be discussed. In fact, as previously described, laminar premixed flames have characteristic propagation speed, $S_f$, and thickness, $\delta_t$. The problem is more difficult in non-premixed turbulent combustion because diffusion flames do not propagate and, accordingly, exhibit no intrinsic characteristic speed. Moreover, the thickness of the flame depends on the thickness of the local mixing layer developing between fuel and oxidizer and no fixed reference length scale can be defined. This difficulty is well illustrated in the literature, where various characteristic scales have been retained, depending on the authors, (Bilger 1988; Bray and Peters 1994; Lee 1994; Cook and Riley 1996).
5.2 Turbulent premixed combustion diagram

The objective is to analyze premixed turbulent combustion regimes by comparing turbulence and chemical characteristic length and time scales. This analysis leads to combustion diagrams where various regimes are represented as a function of various dimensionless numbers as proposed by many authors: Bray (1980), Borghi (1985, 1998), Williams (1985), Peters (1986, 1999). These diagrams could be a support to select and develop relevant combustion models for a given situation. We present here a formalism combining the recent analysis by Borghi and Destrian (1998) and Peters (1999).

For turbulent premixed flames, the chemical time scale, \( \tau_c \), may be estimated as the ratio of the thickness \( \delta_t \) and the propagation speed \( S_L \) of the laminar flame\(^2\). Estimating the turbulent time from turbulent integral scale characteristics (\( \tau_r = l_t/u' \)), the Damköhler number becomes:

\[
Da = \frac{\tau_r}{\tau_c} = \frac{l_t}{\delta_t} \frac{S_L}{u'} \tag{5.3}
\]

where a velocity ratio \( (u'/S_L) \) and a length scale ratio \( (l_t/\delta_t) \) are evidenced.

5.2.1 Combustion regimes

For large values of the Damköhler number \( (Da \gg 1) \), the flame front is thin and its inner structure is not affected by turbulence motions which only wrinkle the flame surface. This *flamelet regime* or *thin wrinkled flame regime* (Fig. 9a) occurs when the smaller turbulence scales (i.e. the Kolmogorov scales), have a turbulent time \( \tau_k \) larger than \( \tau_c \) (turbulent motions are too slow to affect the flame structure). This transition is described in term of the Karlovitz number \( K_a \):

\[
K_a = \frac{\tau_c}{\tau_k} = \frac{l_k}{l_t} \frac{u_k}{S_L} \tag{5.4}
\]

The size \( l_k \) and the velocity \( u_k \) of Kolmogorov structures are given by:

\[
l_k = \left( \frac{\nu^3}{\varepsilon} \right)^{\frac{1}{4}} ; \quad u_k = (\nu \varepsilon)^{1/4} \tag{5.5}
\]

where \( \varepsilon \) is the dissipation of the turbulent kinetic energy \( k \). As the integral length scale \( l_t \) may be written:

\[
l_t = \left( \frac{u'^3}{\varepsilon} \right) \tag{5.6}
\]

\(^2\)This chemical time \( \tau_c \) corresponds to the time required for the flame to propagate on a distance equal to its own thickness. But this time may also be viewed as a diffusive time scale, using Eq. (3.1):

\[
\tau_c = \frac{\delta_t}{S_L} = \frac{1}{Re_l} \frac{\delta_t}{\nu}
\]
we have:

\[ Ka = \left( \frac{u'}{S_L} \right)^{\frac{3}{2}} \left( \frac{l_f}{\delta_i} \right)^{-\frac{1}{2}} \]  

(5.7)

where \( \nu = \delta_i S_L \), corresponding to an unity flame Reynolds number \( Re_f \), has been used (Eq. 3.1).

Reynolds, \( Re \), Damköhler, \( Da \), and Karlovitz, \( Ka \), numbers are related as:

\[ Re = Da^2 Ka^2 \]  

(5.8)

The Karlovitz number also compares the flame and the Kolmogorov length scales according to:

\[ Ka = \left( \frac{\delta_i}{l_k} \right)^2 \]  

(5.9)

The Karlovitz number is used to define the Klimov-Williams criterion, corresponding to \( Ka = 1 \), to delineate between two combustion regimes. This criterion was first interpreted as the transition between the flamelet regime \( (Ka < 1) \), previously described, and the distributed combustion regime where the flame structure is strongly modified by turbulence motions. In a recent analysis, Peters (1999) has shown that, for Karlovitz numbers larger than unity \( (Ka > 1) \), turbulent motions become able to affect the flame inner structure but not necessarily the reaction zone. This reaction zone, where heat is released, has a thickness \( \delta_r \), quite lower that the thermal thickness \( \delta_i \) of the flame \( (\delta_r \approx 0.1 \delta_i) \). The Karlovitz number based on this reaction thickness is:

\[ Ka_r = \left( \frac{\delta_r}{l_k} \right)^2 \approx \frac{1}{100} \left( \frac{\delta_i}{l_k} \right)^2 \approx \frac{Ka}{100} \]  

(5.10)

Then, Peters (1999) proposes the following turbulent premixed flame regimes:

- **\( Ka < 1 \): flamelet regime or thin wrinkled flame regime** (Fig. 9a). Two subdivisions may be proposed depending on the velocity ratio \( u'/S_L \):
  
  - \( (u'/S_L) < 1 \): wrinkled flame. As \( u' \) may be viewed as the rotation speed of the larger turbulent motions, turbulent structures are unable to wrinkle the flame surface up to flame front interactions. The laminar propagation is predominant and turbulence / combustion interactions remain limited.
  
  - \( (u'/S_L) > 1 \): wrinkled flame with pockets ("corrugated flames"). In this situation, larger structures become able to induce flame front interactions leading to pockets.

- **\( 1 < Ka \leq 100 \) (\( Ka_r < 1 \)): thickened wrinkled flame regime or thin reaction zone.** In this case, turbulent motions are able to affect and to thicken the flame preheat zone but cannot modify the reaction zone which remains thin and close to a laminar reaction zone (Fig. 9b).
• $Ka > 100$ ($Ka_r > 1$): **Thickened flame regime or well-stirred reactor.** In this situation, preheat and reaction zones are strongly affected by turbulent motions and no laminar flame structure may be identified (Fig. 9c).

These various regimes are generally displayed on a logarithmic diagram ($u'/S_L ; l_r/\delta_l$), similar to the one presented on Fig. 10.

### 5.2.2 Comments

This analysis, leading to a rough classification of combustion regimes as a function of characteristic numbers, has been developed as a support to derive and choose turbulent combustion models. Following this classification, most practical applications correspond to flamelet or thickened wrinkled flame regimes. Nevertheless, such analysis are only qualitative and should be used with care. A diagram such as the one displayed on Fig. 10 cannot be used to determine the combustion regime of a practical system from $(u'/S_L)$ and $(l_r/\delta_l)$ ratios:

- The analysis is based on the assumption of an homogeneous and isotropic turbulence, unaffected by heat release which is probably wrong in practical situations.

- Some used quantities are not clearly defined. For example, the flame thickness $\delta_l$ may be based on the thermal thickness or on the diffusive thickness corresponding to unity flame Reynolds number ($\delta_l S_L/\nu \approx 1$). Accordingly, the limits between the various regimes may noticeably change.

- All regime limits are based on order of magnitude estimations and not on precise derivations. For example, the flamelet regime limit could correspond to a Karlovitz number $Ka = 0.1$ or $Ka = 10$, rather than $Ka = 1$.

- Various effects are not taken into account here. For example, viscous effects are neglected. Kolmogorov vortices are the most efficient in term induced strain rate but, because of viscous dissipation, have a short lifetime and therefore only limited effects on combustion. Unsteady effects play also an important role neglected here. Darabiha (1992) has shown that a strained laminar flame may sustain strain rates stronger than the extinction strain rate during a limited amount of time. Turbulent motions also induce flame curvature effects leading to a flame stronger than a planar flame.

Poinset et al. (1991) have analyzed turbulent premixed combustion diagrams using direct numerical simulations of flame / vortex interactions. Without providing more details about this analysis, let us point out that the flamelet regime seems to extend over the Klimov-Williams criterion (see Fig. 10). In fact, an essential mechanism revealed by DNS is that small turbulent scales, which are supposed in classical theories to have the strongest effects on flames, have small lifetimes because of viscous dissipation and therefore only limited
Figure 9: Turbulent premixed combustion regimes as identified by Borghi and Destriau (1995). (a) Flamelet (thin wrinkled flame). (b) Thickened wrinkled flame regime. (c) Thickened flame regime.
Figure 10: Turbulent premixed combustion diagram (Borghi and Destriau 1998; Peters 1997). Combustion regimes are identified using the length scale \( l_t/\delta_t \) and the velocity \( u'/S_L \) ratios. The Klimov-Williams criterion \( (K_u = 1) \) corresponds to a flame thickness \( \delta_t \), equal to the Kolmogorov scale \( l_k \). Below this line, the flame is thinner than any turbulent scale. Below the line delineating the Peters criterion \( (K_u = 100 \text{ or } K_u = 1) \), the reaction zone thickness, \( \delta_r \), is thinner than any turbulent scale and is not affected by turbulent motions (the criterion is plotted assuming \( \delta_r \approx 0.1 \delta_t \)). The flamelet regime limit devised by Poinset et al. (1991) from direct numerical simulations is also displayed. The criterion proposed by Veynante et al. (1997) to delineate between gradient (above) and counter-gradient (below) turbulent transport is displayed assuming a heat release factor \( \tau = T_b/T_u - 1 = 6 \) where \( T_u \) and \( T_b \) are respectively the fresh and the burnt gases temperature (see § 8).
effects on combustion. Roberts et al. (1993) have recovered experimentally these results. Peters (1999) shows that his criterion $K_u = 100$ (i.e. $K_u = 1$) is in quite good agreement with the transition proposed by Poinset et al. (1991), at least when the length scale ratio, $l_c/l_t$, is sufficiently high.

All these analysis are implicitly based on a single step irreversible reaction. In actual combustion, a large number of chemical species and reactions have to be included (several hundred species and several thousand reactions for propane burning in air). These reactions may correspond to a large range of chemical time scales. For example, the propane oxidation may assumed to be fast compared to turbulent time scale. On the other hand, the $CO_2$ formation from carbon monoxide (CO) and $OH$ radical in the burnt gases is quite slower with chemical time of the same order than turbulent times.
The mean heat release rate is the main quantity of practical interest in combusting flows and should, at least, be predicted by turbulent combustion models. The simplest and more direct approach is to develop the chemical rate in Taylor series as a function of species mass fractions and temperature but this analysis is limited by its low accuracy and by the rapidly growing complexity of the chemistry (§ 4). Therefore, the non-linear character of the chemistry requires the introduction of new tools.

These new tools must be designed to describe turbulent flames, and have to provide estimation of mean production or consumption rates of chemical species. They also have to be based on known quantities (mean flow characteristics, for example) or from quantities that may be easily modeled or estimated from balance equations. In this section, a generic description of the main concepts proposed to model turbulent combustion is proposed. The relations between the various approaches is also emphasized but the closure strategy will be presented in the subsequent sections.

The basic ingredients to describe turbulent flames remain the quantities introduced for laminar flame analysis: the progress variable $c$ for premixed combustion ($c = 0$ in fresh gases and $c = 1$ in burnt gases, see § 3.1), and, the mixture fraction $Z$ for non-premixed flames ($Z$ is a passive scalar, with $Z = 0$ in pure oxidizer and $Z = 1$ in pure fuel, § 3.2). Under a flamelet assumption, the flame surface may be related to the location of the maximum heat release. This surface corresponds to $c = c_{fl}$ in premixed combustion and to $Z = Z_{st}$ in non-premixed flames. More generally, the flame corresponds to values of the progress variable $c$ lying between 0 and 1 ($0 < c < 1$) or to the vicinity of $Z = Z_{st}$. Accordingly, description of the turbulent flames, assuming a simple chemistry, are therefore mainly based on $c$ or $Z$ scalar fields. As the balance equations for $c$ (Eq. 3.3) and $Z$ (Eq. 3.6) are similar, except for the chemical source term added to the $c$-equation, all approaches will be devised for premixed turbulent flames, using the progress variable $c$. In non-premixed flames, $c$ is replaced by the mixture fraction $Z$ and the reaction term vanishes.

Three main types of analysis, corresponding to three points of view are usually performed to describe turbulent combustion:

- **In the geometrical analysis**, the flame is described as a geometrical surface, this approach is usually linked to a flamelet assumption (the flame is thin compared to the flow scales). Following this view, scalar fields ($c$ or $Z$) are studied in terms of iso-value surfaces (iso-$c_{fl}$ or iso-$Z_{st}$).

- **The statistical properties** of scalar fields may be collected and analyzed for any location within the flow. Mean values of various parameters are then extracted using
the probability of finding a particular set of values of a concentration species or temperature.

- A mixing description. Under a flamelet assumption (large Damköhler numbers, see section 5), the reaction rate is mainly limited by the turbulent transport and mixing (the chemical reaction is assumed to be fast enough). The mean reaction rate is then quantified in terms of turbulent mixing, estimated from the mean scalar dissipation rate.

6.1 Geometrical description

The flame front is here described as a geometrical entity. This analysis is generally linked to the assumption of a sufficiently thin flame, which is then viewed as an interface between fresh and burnt gases in premixed combustion or as an interface between fuel and oxidizer in non-premixed situations.

6.1.1 Level-set approach: $G$-field equation

The balance equation for the mean progress variable is written:

$$\frac{\partial \bar{\mathcal{G}}}{\partial t} + \bar{u} \cdot \nabla \bar{\mathcal{G}} = S_T \left| \nabla \bar{\mathcal{G}} \right|$$

(6.1)

where $S_T$ is the turbulent flame speed, to be modeled. This equation describes the propagation of a $G$-field with a given turbulent flame speed $S_T$.

The mean turbulent flame brush is then located at the points where $\bar{\mathcal{G}} = G_0$. The overall turbulent flame is only viewed as a propagating surface without taking into account the flame structure. Accordingly, this formalism is well-suited to numerical simulation of large practical systems where the knowledge of the internal structure of the flame brush is not required. For example, Smiljanovski et al. (1997) have numerically simulated the propagation of a premixed flame over obstacles in a $35 \times 2.25 \times 2.5$ m channel. Nevertheless, a model has to be supplied for $S_T$.

From an experimental point of view, the turbulent flame speed is relatively easy to measure but required the knowledge of the flame front position and of the velocity field ($S_T$ is the displacement speed of the flame front relatively to the unburnt gases flow field).

6.1.2 Flame surface density description

The flame is identified as a surface and the flame surface density (i.e. the available flame area per unit volume), $\Sigma$, is introduced. The mean burning rate of a species $i$ is then
Figure 11: Flame surface density modeling

modeled as:

$$\bar{w}_i = Q_i \Sigma$$  \hspace{1cm} (6.2)

where $\tilde{Q}_i$, is the mean local burning rate per unit of flame area and is related to the properties of the local flame front, integrated along the normal direction to the flame surface. $Q_i$ is generally estimated from a prototype flame, incorporating more or less complexity. For instance, ones may consider a planar laminar flame, submitted or not to a steady strain, a laminar flame where curvature effects have been introduced, or even a laminar unsteady strained and curved flame. The main advantage of this formulation, summarized on Fig. 11, is to decouple the chemistry description $(Q_s)$ from the flame/turbulence interaction $(\Sigma)$. In fact, the flame surface is convected, diffused, curved and strained by the velocity field (Fichot et al. 1993; Trouvé and Poinset 1994).

The flame surface density $\Sigma$ may be estimated either from algebraic relations (see § 7.4.1.) or as a solution of a balance equation. Such a balance equation has been first proposed by Marble and Broadwell (1977) for non-premixed turbulent flames, from phenomenological analysis. Then, recent works have developed a more rigorous derivation from geometrical considerations (Candel and Poinset 1990; Trouvé and Poinset 1994) or a statistical description (Pope 1988a; Vervisch et al. 1995; Van Kaisment and Veynante 1998) leading to an exact, but unclosed, balance equation. This equation may be written:

$$\frac{\partial \Sigma}{\partial t} + \nabla \cdot ((\mathbf{u})_{\Sigma} \Sigma) = \nabla \cdot (\mathbf{u})_{\Sigma} \nabla \Sigma - \nabla \cdot [(\mathbf{w} \nabla \cdot \mathbf{n})_{\Sigma}] + \langle \mathbf{w} \nabla \cdot \mathbf{n} \rangle_{\Sigma}$$  \hspace{1cm} (6.3)
where \( \mathbf{n} \) is the unit vector normal to the \( c - c^* \) surface and pointing towards the fresh gases \((\mathbf{n} = -\nabla c/|\nabla c|)\). \( \nabla \cdot \mathbf{n} \) corresponds to the flame front curvature. The surface averaged quantity \( Q \), \( \langle Q \rangle_x \), is defined as:

\[
\langle Q \rangle_x = \frac{Q \langle |\nabla c| \delta(c - c^*) \rangle}{\langle |\nabla c| \delta(c - c^*) \rangle}
\]

where \( \Sigma = \langle |\nabla c| \delta(c - c^*) \rangle \) is the flame surface density of \( c - c^* \) surface and \( \delta(c - c^*) \) denotes the Dirac function. The LIRS terms in Eq. (6.3) correspond to unsteady effects and to the flame surface convection, which may be split into a mean and a turbulent contributions according to \((u)_s = \bar{u} + (u')_s\). The first term in the RIRS expresses the action of the tangential strain rate on the flame surface. The last two terms correspond to front convection due to a normal propagation and combined propagation/curvature effects.

Flame surface density may be extracted from flame front or reaction rate visualizations (tomographic imaging, laser induced fluorescence, ...). But, such visualizations are generally two-dimensional and some assumptions on the third direction are required to estimate \( \Sigma \).

6.2 Statistical approaches: Probability density function

Even though the \( C \) field and the density of flame surface \( \Sigma \) need some statistical treatments, they are initially based on a geometrical view of the flame. One point statistical approaches, without background thinking of interfaces and flame structure, are also widely retained to describe turbulent flow fields.

6.2.1 Probability density function (pdf)

A statistical description of the flow field may be founded on probability density functions (PDF). Defining the probability density function \( P(\Psi_1, \Psi_2, ..., \Psi_N) \) as:

\[
\text{Probability } (\Psi_1 < Y_1 < \Psi_1 + d\Psi_1, ..., \Psi_N < Y_N < \Psi_N + d\Psi_N) = P(\Psi_1, ..., \Psi_N) d\Psi_1 d\Psi_2 ... d\Psi_N
\]

for a given location, with the normalization relation:

\[
\int_{\Psi_1, \Psi_2, ..., \Psi_N} P(\Psi_1, \Psi_2, ..., \Psi_N) d\Psi_1 d\Psi_2 ... d\Psi_N = 1
\]

where \( Y_1, Y_2, ..., Y_N \) are the thermochemical variables (mass fractions, temperature, ...), any averaged quantity \( \bar{Q} \), for example the species mass fractions or the mean reaction rate \( \bar{\omega}_k \), may be determined as:

\[
\bar{Q} = \int_{\Psi_1, \Psi_2, ..., \Psi_N} Q(\Psi_1, ..., \Psi_N) P(\Psi_1, \Psi_2, ..., \Psi_N) d\Psi_1 d\Psi_2 ... d\Psi_N
\]
This stochastic description has many theoretical advantages. Probability density functions may be defined in any turbulent reacting flow field without any hypothesis. These functions may also be extracted from experimental data or direct numerical simulations. Two main paths are available to determine $P(\Psi_1, \Psi_2, \ldots, \Psi_N)$:

**Presumed probability density functions.** In this approach, the shape of the PDF is a priori assumed (Borghi 1985). The probability density function $p(c)$, where $c$ is the progress variable, is generally supposed to depend only on the mean progress variable $\bar{c}$ and its variance $\tilde{c}^2$ as a $\beta$-function:

$$p(c) = \frac{1}{B(a, b)} c^{a-1} (1 - c)^{b-1} \quad \text{with} \quad B(a, b) = \int_0^1 c^{a-1} (1 - c)^{b-1} \, dc$$

(6.8)

The PDF parameters $a$ and $b$ are determined from $\bar{c}$ and $\tilde{c}^2$ as:

$$a = \bar{c} \left( \frac{1}{\tilde{c}^2} - 1 \right) \quad ; \quad b = \frac{a}{\bar{c}} - a$$

(6.9)

This simplified approach is used in some industrial simulations. Additional balance equations for fluctuating quantities $\tilde{c}^2$ have to be modeled and solved.

**Transport equation for the probability density function $P$.** An exact transport equation for PDF may be derived (Pope 1985; Dopazo 1994):

$$\rho \frac{\partial \tilde{P}}{\partial t} + \rho U_k \frac{\partial \tilde{P}}{\partial x_k} = - \left\{ \frac{\partial}{\partial x_k} \left[ \tilde{P} \left( \overline{U_i Y_j} \Psi \right) \tilde{P} \right] \right\}$$

Turbulent convection

$$- \left\{ \tilde{P} \sum_{i=1}^{N} \sum_{j=1}^{N} \frac{\partial}{\partial \Psi_i} \frac{\partial}{\partial \Psi_j} \left[ D \left( \frac{\partial Y_i}{\partial x_k} \frac{\partial Y_j}{\partial x_k} | Y = \Psi \right) \tilde{P} \right] \right\}$$

Molecular mixing

$$- \left\{ \tilde{P} \sum_{i=1}^{N} \frac{\partial}{\partial \Psi_i} \left( \omega_i (\Psi_1, \Psi_2, \ldots, \Psi_N) \tilde{P} \right) \right\}$$

Chemical reaction

(6.10)

where $\overline{QY = \Psi}$ correspond to conditional averaging of quantity $Q$ for the sampling values $\Psi_i$.

The reaction term of this equation is closed and does not require any modeling but the modeling of the unclosed mixing diffusion term is not obvious. The numerical solution of the PDF-equation is generally based on Monte-Carlo algorithms and is very time consuming. The
above PDF balance equation (6.10) involves only thermochemical quantities. In a more refined approach, joint velocity-thermochemical variables probability density functions may be considered leading to a more complex transport equation.

Probability density functions may be easily extracted from experiments by a statistical analysis of single shot local data (Rayleigh and/or Raman diffusion, Coherent Anti-Stokes Raman Scattering (CARS)....).

6.2.2 Conditional Moment Closure (CMC)

The CMC model, proposed by Klimenko (1990) and Bilger (1993), introduces conditional averaging to focus on particular states between fresh gases and fully burnt product in premixed flames, or, between fuel and oxidizer in non-premixed combustion. In premixed flames, the conditional quantity is the progress variable \( c \), whereas for non-premixed combustion, the mixture fraction is used (Bilger 1993). In premixed flames, the mean value, \( \tilde{Y} \), of any quantity \( Y \) is estimated as:

\[
\tilde{Y} = \frac{1}{\tilde{P}(c^*; \mathbf{x}, t)} \int_0^1 (Y|c = c^*) \tilde{P}(c^*; \mathbf{x}, t) \, dc^* \tag{6.11}
\]

Klimenko (1990) and Bilger (1993) have proposed to solve balance equation for the conditional quantities \( Q_i(c^*) \) defined as (Chen and Kollmann 1994):

\[
Q_i(c^*) = \frac{(\rho \bar{Y}_i | c = c^*)}{(\rho c = c^*)} \tag{6.12}
\]

Despite this formalism has been derived from a statistical analysis, this approach may also be viewed as a multi-surface formalism. Any conditional quantity \( (Y|c = c^*) \) corresponds to the conditional average of \( Y \) along the iso-surface \( c = c^* \).

6.3 Mixing description approaches

6.3.1 Scalar dissipation rate

As discussed in section 3, under the so-called flamelet assumption, corresponding to large Damköhler numbers, the reaction rate in turbulent combustion is mainly limited by turbulence time scales. The idea is then to quantify this reaction rate in terms of turbulent mixing. In premixed flames, the turbulence mixing may be related to the variance \( c^2 \) of the progress variable \( c \).
A balance equation for the variance \( \tilde{c}^2 \) may be easily derived from the instantaneous equation \( c \), leading to:

\[
\frac{\partial \rho \tilde{c}^2}{\partial t} + \nabla \cdot (\rho \bar{u} \tilde{c}^2) + \nabla \cdot (\rho \bar{u} \tilde{c}^2) = \nabla \cdot (\rho D \nabla \tilde{c}^2) + 2 \nabla \cdot (\rho D \tilde{c} \nabla \tilde{c}) + 2 \nabla \cdot (\rho D \tilde{c} \nabla \tilde{c}) - \frac{2 \rho D \tilde{c} \cdot \nabla \tilde{c}}{\bar{\rho} \bar{D} \nabla \bar{c} \cdot \nabla \bar{c}} \quad (6.13)
\]

Accordingly to this balance equation, the scalar dissipation rate \( \bar{\chi} = \rho D \nabla \bar{c} \cdot \nabla \bar{c} \) represents the speed at which the fluctuations \( \tilde{c}^2 \) are consumed by viscous dissipation and turbulent transport. Therefore \( \bar{\chi} \) directly measures the mixing of the reactants. Accordingly, assuming a fast chemistry and a combustion limited by mixing, the scalar dissipation rates of the mixture fraction \( Z \) for non-premixed flame or the scalar dissipation rate of the progress variable \( c \) for premixed combustion, naturally appear as interesting ingredients to express mean burning rates (see § 6.4).

The scalar dissipation rate may be estimated from algebraic closures (Peters 1986; Bilger 1989; Bray 1996) or from a modeled balance equation (Mantel and Borghi 1994). But, despite some attempts, scalar dissipation rates are very difficult to achieve in experiments. In fact, measurements have to be based on processing of scalar field imaging (laser tomography, Rayleigh diffusion, laser induced fluorescence,...), extracting the square of the local instantaneous scalar gradient (in 3D !). Accordingly, uncertainties may become very large, blurring any analysis.

6.4 Similarities and links between the tools

Major links between the tools developed above are now discussed. Without loss for the generic character of the discussion, we consider the case of a turbulent premixed flame represented with the progress variable \( c \). This turbulent flame may be described using three variables, corresponding to three different approaches:

- The pdf of the progress variable \( \bar{P}(c^*; \bar{c}, t) \).
- The density of flame surface \( \Sigma \).
- The scalar dissipation rate of the progress variable \( \bar{\chi} = \rho D \nabla \bar{c} \cdot \nabla \bar{c} \).

Two key relations provide links between these quantities. First, the Dirac \( \delta \) function is an instantaneous measure of the probability density function \( \bar{P}(c^*; \bar{c}, t) \).

\[
\bar{P}(c^*; \bar{c}, t) = \delta (c(c^*; \bar{c}, t) - c^*)
\quad (6.14)
\]

---

\(^3\)Various definitions of the scalar dissipation rate may be found in the literature, including the density \( \rho \) or a factor \( \lambda \); instantaneous (\( c \)) or fluctuating (\( c^* \)) values of the concentration species. In fact:

\[
\bar{\chi} = \rho D \nabla \bar{c} \cdot \nabla \bar{c} = \rho D \nabla \bar{c} \cdot \nabla \bar{c} + 2 \rho D \nabla \bar{c} \cdot \nabla \bar{c} + \rho D \nabla \bar{c} \cdot \nabla \bar{c}
\]

When mixing in an homogeneous field is considered (no \( \nabla \bar{c} \) gradient), the scalar dissipation reduces to \( \rho D \nabla \bar{c} \cdot \nabla \bar{c} \).
Pope (1988b) has also shown that the density $\Sigma^*$ of the iso-surface $c = c^*$ is exactly defined by:

$$\Sigma^*(x, t) = |\nabla c| \delta(c - c^*) = \left( |\nabla c| \right) \overline{P(c^*; x, t)}$$  \hspace{1cm} (6.15)

and depends on the gradient of the progress variable $c$ conditioned on the surface $c = c^*$ and on the probability to have $c = c^*$. This relation has been further investigated by Vervisch et al. (1993) for premixed flames and by Van Kalnithout and Veynaute (1998) for non-premixed flames. Relation (6.15) exhibits strong similarities between the pdf $\overline{P(c^*; x, t)}$ and $\Sigma$ and may be used to derive an exact balance equation for $\Sigma$ from the time evolution of the scalar field $c$ as described in § 6.1.2 (This transport equation may also be obtained from geometrical considerations).

Under a flamelet assumption (thin flame front), the mean scalar dissipation $\bar{\chi}$ may be estimated as:

$$\bar{\chi} = \rho D \nabla c \cdot \nabla c \approx \rho D |\nabla c| |\nabla c| \delta(c - c^*) = \langle \rho D |\nabla c| \rangle^* \Sigma^*$$  \hspace{1cm} (6.16)

where $\langle Q \rangle^*$ denotes an averaging along the $c = c^*$ surface.

According to these relations, probability density functions, flame surface density and scalar dissipation concepts are strongly related (see Fig. 12). This implies that the turbulent combustion models proposed using one or the other of these quantities have strong similarities, and may only differ in the closure schemes introduced in the balance equations.
Flame surface density

\[ \Sigma = |\nabla c|_{c^*} \rho(c^*) \]

CMC

Turbulent combustion

Probability density function

\[ p(c^*) \]

Scalar dissipation

\[ \bar{\chi} = 2\rho D|\nabla c||\nabla c| \]

Figure 12: Relations between tools for turbulent combustion modeling.
7 Reynolds-averaged models for turbulent premixed combustion

7.1 Turbulent flame speed

Turbulent premixed flames may be described in terms of a global turbulent flame speed \( S_T \) (see § 3.3.1 and 6.1.1). From experimental data (Abdel-Gayed et al. 1984; Abdel-Gayed and Bradley 1989) or theoretical analysis (Renormalization Group Theory, Yakhot et al. 1992), the following expression has been proposed:

\[
\frac{S_T}{S_L} = 1 + \alpha \left( \frac{u'}{S_L} \right)^n
\]  

(7.1)

where \( \alpha \) and \( n \) are two model constants close to unity, \( u' \) is the turbulent velocity (i.e. the RMS velocity).

Unfortunately, the turbulent flame speed \( S_T \) is not a well-defined quantity (Gouldin 1995). Experimental data exhibit a large scatter and depend on various parameters (chemistry characteristics, turbulence scales, flow geometry,...). While this global approach is not well suited to close Favre averaged transport equations, it may be of interest in the context of Large Eddy Simulations (§ 10).

7.2 Eddy-Break-Up model

Devised by Spalding (1971), this model is based on a phenomenological analysis of turbulent combustion assuming high Reynolds (Re \( \gg \) 1) and Damköhler (Da \( \gg \) 1) numbers. The reaction zone is viewed as a collection of fresh and burnt gas pockets. Following the Kolmogorov cascade, turbulence leads to a break down of fresh gases structures. Accordingly, the mean reaction rate is mainly controlled by the turbulent time \( \tau_r \). When oxidizer is in excess, the mean reaction rate is expressed as:

\[
\overline{\omega_f} = -C_{EBU} \overline{Y_f} \sqrt{Y_{f\phi}} \frac{Y_f}{\tau_{EBU}}
\]  

(7.2)

where \( Y_{f\phi} \) denotes the fuel mass fraction fluctuations and \( C_{EBU} \) is a model constant of the order of unity. The turbulence time \( \tau_r \) is estimated from the turbulence kinetic energy \( k \) and its dissipation rate \( \varepsilon \) according to:

\[
\tau_{EBU} = \frac{k}{\varepsilon}
\]

which is the characteristic time of the integral length scales of the turbulent flow field. Then, the Eddy-Break-Up is generally used together with the \( k-\varepsilon \) turbulence model.
Mass fraction fluctuations $\overline{\chi_Y}^2$ must be modeled and may be estimated from a balance equation. A first simplified analysis leads to the very simple result:

$$\overline{\omega_f} = -\frac{V_{EBU}}{k} \frac{\varepsilon}{Y_F} \left( 1 - \frac{Y_f}{Y_F} \right)$$

(7.3)

where $Y_F$ is the initial fuel mass fraction in the reactant stream.

This model is attractive because the reaction rate is simply written as a function of known quantities without any additional transport equation. Accordingly, the Eddy-Break-Up model may be found in most industrial codes and practical applications. Nevertheless, the modeled reaction rate does not depend on chemical characteristics and assumes an homogeneous and isotropic turbulence. Some adjustments of the model constant $C_{EBU}$ have been proposed to incorporate chemistry features (Said and Borghi 1988). The Eddy-Break-Up model also tends to overestimate the reaction rate, especially in highly strained regions, when the ratio $\varepsilon/k$ is large (flame-holder wakes, walls,...).

### 7.3 Bray-Moss-Libby (BML) model

#### 7.3.1 Introduction

Known under the initials of its authors, Bray, Moss and Libby, this model, first proposed in 1977, has been the subject of a large amount of works leading to many improvements (see papers by Bray, Moss and Libby, and then by Bray, Champion et Libby). Combining a statistical approach using probability density functions and a physical analysis, this model has evidenced some special features of turbulent premixed combustion (counter-gradient turbulent transport, flame turbulence generation,...). Our presentation will be mainly limited to basic concepts of the BML formulation.

A one-step, irreversible chemical reaction between two reacting species, fresh gases ($R$) and combustion products ($P$) is considered:

$$R \rightarrow P$$

Most classical assumptions are made to simplify the model formulation: perfect gases, incompressible flows, constant chemical properties, unity Lewis numbers,...). A progress variable, $c$ of the chemical reaction is introduced and is such that $c = 0$ in fresh gases and $c = 1$ in fully burnt gases, as described in Section 3.1.

The basic idea of the BML formulation is to write the probability density function of the progress variable $c$ at a given location $x$ as a sum of fresh, fully burnt and burning gases contributions (Fig. 13):

$$P(c, x) = \alpha(x) \delta(c) + \beta(x) \delta(1 - c) + \gamma(x) f(c; x)$$

(7.4)

fresh gases    burnt gases    burning gases
where \( \alpha, \beta \) and \( \gamma \) respectively denotes the probability to have, at location \( x \), fresh gases, burnt gases and reacting mixture, \( \delta(c) \) and \( \delta(1 - c) \) are respectively the Dirac delta functions corresponding to fresh gases \( (c = 0) \) and fully burnt ones \( (c = 1) \).

Normalization of the probability density function:

\[
\int_0^1 P(c, x) \, dc = 1
\]  

(7.5)

leads to the following relations:

\[
\alpha + \beta + \gamma = 1
\]  

(7.6)

\[
\int_0^1 f(c, x) \, dc = 1
\]  

(7.7)

with, of course, \( f(0) = f(1) = 0 \).

The balance equation for the progress variable \( c \) may be written:

\[
\frac{\partial \rho c}{\partial t} + \nabla \cdot (\rho uc) = \nabla \cdot (\rho D \nabla c) + \dot{\omega}
\]  

(7.8)

This equation is averaged and the mean reaction rate, at the location \( x \) is:

\[
\bar{\omega}(x) = \int_0^1 \dot{\omega}(c) P(c, x) \, dc
\]  

(7.9)

leading to (7.4):

\[
\bar{\omega}(x) = \gamma(x) \int_0^1 \dot{\omega}(c) f(c, x) \, dc
\]  

(7.10)

All studies about this line of models are based on this formulation. The objective is now to determine the unknown functions \( \alpha, \beta, \gamma \) and the probability density function \( f \).
Figure 14: Intermittency between fresh and fully burnt gases at a location $x$ in the reaction zone. This signal corresponds to a bimodal ($c = 0$ and $c = 1$) probability density function.

### 7.3.2 BML model analysis

This model is developed under the assumption that $Re \gg Da \gg 1$, corresponding to $\gamma \ll 1$. At a given location in the flow, an intermittency between fresh gases ($c = 0$) and fully burnt ones ($c = 1$) is observed and the probability density function of the progress variable $c$ reduces to:

$$P(c, x) = \alpha(x)\delta(c) + \beta(x)\delta(1 - c)$$  \hspace{1cm} (7.11)

At a given location $x$ inside the reaction zone, $c$ looks like a telegraphic signal as displayed in Fig. 14.

Under this assumption, the $\alpha$ and $\beta$ functions are easily determined as a function of the Favre average progress variable $\bar{c}$:

$$\overline{\rho c} = \rho \bar{c} = \int_0^1 \rho c P(c) dc = \rho_b \beta$$  \hspace{1cm} (7.12)

where $\rho_b$ is the burnt gases density.

$$\beta = \frac{\overline{\rho c}}{\rho_b} \hspace{1cm} \text{and} \hspace{1cm} \alpha = 1 - \frac{\overline{\rho c}}{\rho_b}$$  \hspace{1cm} (7.13)

One may also introduce the reaction heat release factor $\tau$, defined as:

$$\tau = \frac{\rho_u}{\rho_b} - 1 = \frac{T_b}{T_v} - 1$$  \hspace{1cm} (7.14)

The mean density $\overline{\rho}$ is written:

$$\overline{\rho} = \int_0^1 \rho \, dc = \alpha \rho_u + \beta \rho_b = \left(1 - \frac{\overline{\rho c}}{\rho_b}\right) \rho_u + \frac{\overline{\rho c}}{\rho_b} \rho_b$$  \hspace{1cm} (7.15)
leading to:

\[ \rho_u = (1 + \tau) \rho_c = \bar{\rho} (1 + \bar{\tau}) \]  

(7.16)

corresponding to the perfect gases state law, assuming a constant pressure \( \rho \).

Then, the probabilities \( \alpha \) and \( \beta \) become:

\[ \alpha = \frac{1 - \bar{\tau}}{1 + \bar{\tau}} \quad \beta = \frac{(1 + \tau) \bar{\tau}}{1 + \bar{\tau}} \]  

(7.17)

The probability density function \( P(c) \) is completely determined and depends only on the mean progress variable \( \bar{c} \) (and on the heat release factor, \( \tau \), which is constant for a given chemical reaction). The BMG model may be also viewed as a presumed probability density function model. But, the mean reaction rate \( \bar{\omega} \) cannot be determined because the probability \( \gamma \) has been neglected in this analysis (Eq. 7.10). \( \bar{\omega} \) must be estimated from another approach.

From the \( c \)-balance equation (7.8), a balance equation for \( c(1 - c) \) is derived after some mathematical manipulations:

\[ \frac{\partial}{\partial t} [\rho c (1 - c)] + \nabla \cdot [\rho u c (1 - c)] = \nabla \cdot (\rho D \nabla c (1 - c)) + 2 \rho D \nabla c \cdot \nabla c - 2 c \bar{\omega} + \dot{\omega} \]  

(7.18)

Under the assumption of the BMG model, the progress variable \( c \) is equal to zero or to the unity. Accordingly, \( c(1 - c) = 0 \) and the balance equation (7.18) reduces to:

\[ 2 \rho D \nabla c \cdot \nabla c = 2 c \bar{\omega} - \dot{\omega} \]  

(7.19)

leading to, after averaging:

\[ 2 \rho D \nabla c \cdot \nabla c = (2 c_m - 1) \bar{\omega} \]  

(7.20)

where a progress variable \( c_m \), defined as:

\[ c_m = \frac{\int_0^1 \omega f(c) dc}{\int_0^1 \bar{\omega} f(c) dc} \]  

(7.21)

has been introduced and characterizes the chemical reaction.

The mean reaction rate \( \bar{\omega} \) becomes:

\[ \bar{\omega} = \frac{\bar{p}_\lambda}{2 c_m - 1} \]  

(7.22)

where \( \bar{p}_\lambda \) is the scalar dissipation of the progress variable \( c \).

\[ \bar{p}_\lambda = \bar{p}_\lambda = \rho D \nabla c \cdot \nabla c = \rho D \frac{\partial c}{\partial x_i} \frac{\partial c}{\partial x_i} \]  

(7.23)
The mean reaction rate \( \overline{\dot{\omega}} \) is then related to the dissipation rate \( \overline{\chi} \), describing the turbulent mixing, and to \( c_m \), characterizing the chemical reaction. To close the BMI model, a balance equation for \( \overline{\chi} \) could be derived and closed as proposed by various authors. Nevertheless, in a first step, assuming a large turbulence Reynolds number and “small scale dissipation”, one may assumed:

\[
\rho \overline{\chi} = \frac{\overline{\rho e^{\varepsilon^2}}}{\tau_t} \tag{7.24}
\]

where a turbulent time scale, \( \tau_t \) is introduced. Assuming an intermittency between fresh and burnt gases (\( c = 0 \) or \( c = 1 \)), \( \overline{\rho e^{\varepsilon^2}} \) is easily estimated because \( \varepsilon^2 = \overline{\varepsilon}^2 \):

\[
\overline{\rho e^{\varepsilon^2}} = \overline{\rho (\overline{e} - \overline{\varepsilon})^2} = \overline{\varepsilon} \left( \overline{\varepsilon^2} - \overline{\varepsilon}^2 \right) = \overline{\varepsilon} \overline{\varepsilon} (1 - \overline{\varepsilon}) \tag{7.25}
\]

leading to (Eq. 7.22):

\[
\overline{\varepsilon} = \frac{2}{2e_m - 1} \frac{\overline{\rho e^{\varepsilon^2}} (1 - \overline{\varepsilon})}{\tau_t} \tag{7.26}
\]

corresponding to the expression proposed by Spalding in the Eddy-Break-Up model. Accordingly, the BMI model may be viewed as a theoretical derivation, where the assumptions made are clearly stated, of the Eddy-Break-Up (EBU) model, previously based on a phenomenological approach.

### 7.3.3 Reynolds and Favre averaging

Assuming a bimodal distribution of the progress variable \( c \), Reynolds (\( \overline{\cdot} \)) and Favre (\( \overline{\cdot} \)) averages are easily related. From:

\[
\overline{\cdot} = \int_0^1 cP(c) \, dc = \beta \tag{7.27}
\]

\[
\overline{\rho e^{\varepsilon^2}} = \overline{\rho e^{\varepsilon^2}} = \int_0^1 \rho e P(c) \, dc = \rho_b \beta = \rho_b \overline{\varepsilon} \tag{7.28}
\]

and expressions (7.16) and (7.17), one easily obtains:

\[
\overline{\varepsilon} = \frac{(1 + \tau \overline{\varepsilon}) \overline{\varepsilon}}{1 + \tau \overline{\varepsilon}} \tag{7.29}
\]

which, in fact, corresponds to a model for the density / progress variable correlations (Eq. 2.15):

\[
\overline{\rho \varepsilon^2} = -\rho \frac{\tau \overline{\varepsilon} (1 - \overline{\varepsilon})}{1 + \tau \overline{\varepsilon}} \tag{7.30}
\]

Reynolds (\( \overline{\cdot} \)) and Favre (\( \overline{\cdot} \)) averages of the instantaneous progress variable \( c \) are compared on Fig. 15 for various values of the heat release factor \( \tau \). Of course, the discrepancy between the two quantities strongly increase with \( \tau \).
Figure 15: The Reynolds average $\overline{\tau}$ of the progress variable $c$ is plotted as a function of the Favre average $\overline{c}$ for various values of the heat release factor $\tau$, assuming a bimodal distribution ($c = 0$ or $c = 1$) of $c$ (Eq. 7.29).

### 7.3.4 Conditional averaging - Counter-gradient turbulent transport

Assuming intermittency between fresh gases ($c = 0$) and fully burnt gases ($c = 1$) may lead to the introduction of conditional averaging. The Favre average $\overline{Q}$ of any quantity $Q$ may be expressed as a function of the fresh gases ($Q^u$) and fully burnt gases ($Q^b$) conditional averages:

$$\overline{Q} = \rho \overline{\rho} Q = \int_0^1 \rho Q P(c) dc = \alpha \rho_u \overline{Q}^u + \beta \rho_b \overline{Q}^b$$

(7.31)

leading to, using Eq. (7.16) and (7.17):

$$Q = (1-\overline{c}) \overline{Q}^u + \overline{c} \overline{Q}^b$$

(7.32)

where $\overline{Q}^u$ and $\overline{Q}^b$ are defined as:

$$\overline{Q}^u = \int_{-\infty}^{+\infty} Q P(Q, c = 0) dQ$$

$$\overline{Q}^b = \int_{-\infty}^{+\infty} Q P(Q, c = 1) dQ$$

$P(Q, c)$ is the conditional pdf (see § 6.2.1), at a given location $x$, of $Q$ for the given value $c$ of the progress variable.

This analysis is quite interesting as fresh and burnt gases characteristics may be separated. Accordingly, the components $\bar{v}_k$ of the mean velocity vector $\bar{u}$ may be written as a linear
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A combination of the conditional fresh and burnt gases averages:

$$\tilde{u}_i = (1 - \tilde{c}) \bar{u}_i^f + \tilde{c} \bar{u}_i^b$$  \hspace{1cm} (7.33)

Then:

$$\tilde{p} \bar{u}_i^f \tilde{c} = \tilde{p} (\bar{u}_i \tilde{c} - \tilde{u}_i \tilde{c}) = \tilde{p} (\tilde{c} \bar{u}_i^f - \tilde{u}_i \tilde{c}) = \tilde{p} \tilde{c} (1 - \tilde{c}) (\bar{u}_i^f - \tilde{u}_i^f)$$  \hspace{1cm} (7.34)

which is the scalar turbulent flux, generally modeled using a gradient assumption:

$$\tilde{p} \bar{u}_i^f \tilde{c} = \frac{\mu_t}{S_c} \left( \frac{\partial \tilde{c}}{\partial x_i} \right)$$  \hspace{1cm} (7.35)

The two expressions (7.34) and (7.35) may describe opposite fluxes. In a first analysis of a left-traveling one-dimensional turbulent flame, the conditional velocity in the burnt gases, \( \bar{u}_i^b \), is expected to be larger than the conditional velocity in the fresh gases, \( \bar{u}_i^f \), because of thermal expansion. According to Eq. (7.34), the turbulent flux, \( \bar{u}_i^f \tilde{c} \), is expected to be positive. On the other hand, as the mean progress variable gradient is also positive, Eq. (7.35) leads to a negative value of \( \tilde{p} \bar{u}_i^f \tilde{c} \). This situation, denoted as "counter-gradient turbulent transport", a key point in the BML analysis, will be further analyzed (§ 8).

The Reynolds stresses \( \bar{u}_i^f \bar{u}_j^f \) may also be decoupled using the same formalism:

$$4 \tilde{u}_i^f \bar{u}_j^f = (1 - \tilde{c}) \bar{u}_i^f \bar{u}_j^f + \tilde{c} \bar{u}_i^f \bar{u}_j^b + \tilde{c}(1 - \tilde{c})(\bar{u}_i^b - \tilde{u}_i^f)(\bar{u}_j^b - \tilde{u}_j^f)$$  \hspace{1cm} (7.36)

where one may note a weighted mean between the Reynolds stresses in the fresh \( \bar{u}_i^f \bar{u}_j^f \) and in the burnt gases \( \bar{u}_i^f \bar{u}_j^b \). The additive term corresponds to the intermittency between fresh and burnt gases.

7.4 Models based on the flame surface area estimation

Several flame surface density models will be described here. Their derivation and their histories differ, but they are based on similar concepts, described in section § 6.1.2, and lead to very close formulations. All these models assume that the chemical reaction occurs in thin layers separating fresh gases from fully burnt ones (high Damköhler number limit). The reaction zone may be viewed as a collection of laminar flame elements called flamelets.

7.4.1 Algebraic expressions for the flame surface density \( \Sigma \)

Assuming intermittency between fresh and burnt gases (§ 7.3), Bray, Moss, Libby and their coworkers have proposed to describe the mean reaction rate \( \bar{\omega}_c \) as the product of a flame crossing frequency \( \nu \) and a local reaction rate per flame crossing, \( \omega_F \):

$$\bar{\omega}_c = \omega_F \nu$$  \hspace{1cm} (7.37)
This crossing frequency is then derived from a statistical analysis of the telegraph equation because $c(t)$ may be viewed as a telegraphic signal (Fig. 14). Then:

$$\nu = \frac{2 \bar{c}(1 - \bar{c})}{\tilde{T}}$$  \hspace{1cm} (7.38)

where $\tilde{T}$ is a $c$-fluctuation time scale.

This analysis is attractive because the crossing frequency $\nu$ may be easily obtained in experiments, for example, from time-resolved local temperature measurements (thermocouple). On the other hand, the flame surface density $\Sigma$ cannot be so easily determined. Nevertheless, the estimation of the local reaction rate per flame crossing is not obvious...

This model has been then rewritten in term of flame surface density, leading to the algebraic expression (Bray et al. 1989):

$$\Sigma = g \frac{\bar{c}(1 - \bar{c})}{\sigma_y L_y} = \frac{g}{\sigma_y L_y} \frac{1 + \tau}{(1 + \tau \bar{c})^2} (1 - \bar{c})$$  \hspace{1cm} (7.39)

where $g$ is a constant of order unity, $\sigma_y$ a flamelet orientation factor measuring the mean angle of the instantaneous flame front with the $\bar{c}$-surface and assumed to be an universal model constant ($\sigma_y \approx 0.6$). $L_y$ is a flame front wrinkling length scale. A submodel is then required to describe the wrinkling length scale $L_y$, generally assumed to be proportional to the integral length scale $l_i$:

$$L_y = C_i l_i \left( \frac{S_L}{u'} \right)^n$$  \hspace{1cm} (7.40)

where $C_i$ and $n$ are two constants of the order of unity.

The BML model proposes a simple algebraic expression to estimate the flame surface density $\Sigma$ and the corresponding reaction rate, but Bray, Moss, Champion and Libby have mainly focused their attention to a careful description of the turbulent fluxes using the balance equations for the Reynolds stresses $\bar{u}_i u_j$ and the scalar fluxes $\bar{u}_i c''$ to take into account the possible occurrence of counter-gradient transport and the flame turbulence generation.

The flame surface density may be also derived from fractal theories, leading to (Gouldin et al. 1989):

$$\Sigma = \frac{1}{L_{inner}} \left( \frac{L_{outer}}{L_{inner}} \right)^{D-2}$$  \hspace{1cm} (7.41)

where $L_{inner}$ and $L_{outer}$ are respectively the inner and outer cut-off length scales (the flame surface is assumed to be fractal between these two scales). $D$ is the fractal dimension of the flame surface. The cut-off scales are generally estimated for the turbulence Kolmogorov $l_k$ and the integral $l_i$ length scales.
7.4.2 Flame surface density balance equation closures

The previously described balance equation for \( \Sigma \) (Eq. 6.3) is, of course, unclosed and require modeling. The modeled balance equation may be rewritten as:

\[
\frac{\partial \Sigma}{\partial t} + \nabla \cdot (\tilde{U} \Sigma) = \nabla \cdot \left( \frac{\nu}{\sigma_{\Sigma}} \nabla \Sigma \right) + S_1 + S_2 + S_3 - D
\]

(7.42)

where \( S_1, S_2 \) and \( S_3 \) are three source terms and \( D \) is a consumption term. In this expression, the turbulent flux of flame surface density is modeled using a classical gradient assumption, \( \nu \) is the turbulent viscosity and \( \sigma_{\Sigma} \) a flame surface turbulent Schmidt number.

In Table 1 various closures found in the literature are compared. \( S_1 \) term corresponds to the strain rate acting on the surface and induced by the mean flow field. \( S_2 \) is the strain rate due to the turbulent motions and the third source term \( S_3 \) occurs only in the derivation proposed by Mantel and Borghi (1994). \( D \) describes the consumption of flame area. Four main models are summarized here:

These models have strong similarities. For example, the consumption term \( D \) is always proposed to be proportional to \( \Sigma^2 \). A comparison of the ability of these models to predict turbulent flame speed \( \dot{S} \) may be found in Duclos et al. (1993). In recent papers, Prasad and Gore (1999) have compared CPB, CFM1, MB and CD models to predict a turbulent premixed jet flame.

The flame surface density balance equation may be analyzed from direct numerical simulations (Trouvé and Poinso 1994) or on experimental data (Veynante et al. 1994; Veynante et al. 1996).

7.4.3 An example of flame surface density measurements

Flame surface densities may be extracted from experiments as done by Veynante et al. (1994, 1996). The experimental burner is displayed on Fig. 16. A turbulent premixed propane/air flame is stabilized behind a small cylinder (blockage ratio of 6 \%). Flow rates are about 35 to 100 g/s, corresponding to inlet velocities between 10 to 30 m/s (turbulence levels from 5 to 10 \%). Equivalence ratio \( \phi \) are in the range 0.7 to 1.1. Velocity (laser Doppler velocimetry), \( CH \) and \( C_2 \) radical emission (reaction rate estimation) and high-speed laser tomography (flame front characteristics) measurements have been performed and are described in Veynante et al. (1994), Veynante et al. (1996), Duclos (1997), Martel (1998).

Two typical results of flame surface density measurements are displayed in Fig. 17 (half burner). Flame surface density profiles are plotted as a function of the transverse coordinate for various downstream locations. These measurements may be used to analyze flame surface density models (Veynante et al. 1994; Veynante et al. 1996).
<table>
<thead>
<tr>
<th>MODEL</th>
<th>$S_1 = k_m \Sigma$</th>
<th>$S_2 = e_k \Sigma$</th>
<th>$S_3$</th>
<th>$D$</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPB</td>
<td>$A_k \frac{\partial T}{\partial t}$</td>
<td>$\alpha_0 C_4 \left( \frac{\varepsilon}{c} \right)^\frac{3}{2} \Sigma$</td>
<td>$\sigma_0 \frac{U_0^2}{3} \left( \frac{e_k}{c} \right)^{\frac{3}{2}}$</td>
<td>$R = \frac{\gamma_k}{\gamma_k - 1} \frac{\varepsilon}{\varepsilon_0}$</td>
</tr>
<tr>
<td>(Cont et al)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CFM1</td>
<td>$A_k \frac{\partial T}{\partial t}$</td>
<td>$\alpha_0 k \Sigma$</td>
<td>$\beta_0 \frac{U_0^4 + 3 \kappa_k \Sigma^2}{\varepsilon}$</td>
<td>$\frac{\beta_0}{\gamma_k - 1} \left( \frac{E_k}{E_k - 1} \right)^2 \Sigma^2$</td>
</tr>
<tr>
<td>CFM2-a</td>
<td>$A_k \frac{\partial T}{\partial t}$</td>
<td>$\Gamma_k \frac{\varepsilon}{\Theta}$</td>
<td>$\beta_0 \frac{U_0^4 + 3 \kappa_k \Sigma^2}{\varepsilon}$</td>
<td>$\frac{\beta_0}{\gamma_k - 1} \left( \frac{E_k}{E_k - 1} \right)^2 \Sigma^2$</td>
</tr>
<tr>
<td>CFM2-s</td>
<td>$A_k \frac{\partial T}{\partial t}$</td>
<td>$\Gamma_k \frac{\varepsilon}{\Theta}$</td>
<td>$\alpha_0 k \Sigma$</td>
<td>$R = \frac{\gamma_k}{\gamma_k - 1} \frac{\varepsilon}{\varepsilon_0}$</td>
</tr>
<tr>
<td>MB</td>
<td>$E \frac{\partial u}{\partial x} \frac{\partial T}{\partial t}$</td>
<td>$\beta_0 \frac{U_0^4 + 3 \kappa_k \Sigma^2}{\varepsilon}$</td>
<td>$\frac{\beta_0}{\gamma_k - 1} \left( \frac{E_k}{E_k - 1} \right)^2 \Sigma^2$</td>
<td>$\frac{\beta_0}{\gamma_k - 1} \left( \frac{E_k}{E_k - 1} \right)^2 \Sigma^2$</td>
</tr>
<tr>
<td>Mantel-Borgh</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CD</td>
<td>$\alpha_0 A_k \Sigma$</td>
<td>$\kappa \leq \alpha_0 k \frac{U_0}{\varepsilon_k}$</td>
<td>$\beta_0 \frac{U_0^4 + 3 \kappa_k \Sigma^2}{\varepsilon}$</td>
<td>$\frac{\beta_0}{\gamma_k - 1} \left( \frac{E_k}{E_k - 1} \right)^2 \Sigma^2$</td>
</tr>
<tr>
<td>Cheng-Diringer</td>
<td></td>
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</tr>
<tr>
<td>CH1</td>
<td>$\alpha_0 \left( \frac{U_0}{\varepsilon_k} \right) \Sigma$</td>
<td>$\beta_0 \frac{U_0^4 + 3 \kappa_k \Sigma^2}{\varepsilon}$</td>
<td>$\frac{\beta_0}{\gamma_k - 1} \left( \frac{E_k}{E_k - 1} \right)^2 \Sigma^2$</td>
<td>$\frac{\beta_0}{\gamma_k - 1} \left( \frac{E_k}{E_k - 1} \right)^2 \Sigma^2$</td>
</tr>
<tr>
<td>CH2</td>
<td>$\alpha_0 \frac{U_0^4}{\varepsilon_k} \Sigma$</td>
<td>$\beta_0 \frac{U_0^4 + 3 \kappa_k \Sigma^2}{\varepsilon}$</td>
<td>$\frac{\beta_0}{\gamma_k - 1} \left( \frac{E_k}{E_k - 1} \right)^2 \Sigma^2$</td>
<td>$\frac{\beta_0}{\gamma_k - 1} \left( \frac{E_k}{E_k - 1} \right)^2 \Sigma^2$</td>
</tr>
<tr>
<td>Choi-Huh</td>
<td></td>
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</tbody>
</table>

Table 1: Comparison of source ($S_i$) and consumption ($D$) terms in the flame surface density balance equation in different turbulent premixed combustion models (details in text). $k$ and $\varepsilon$ denote respectively the turbulent kinetic energy and its dissipation. $Re_t$ is the turbulent Reynolds number, $Y$ the fuel mass fraction in the case of a lean combustion. $\alpha_0$, $\beta_0$, $\gamma$, $\lambda$, $C_A$, $a_0$, $c$, $C_r$, $E$ and $K$ are model constants. $\Gamma_k$ is the efficiency function in the ITNFS model proposed by (Meneveau and Poinson 1991) and depends on the length scale ($l_l/l_0$) and the velocity ($u'/S_L$) ratio comparing the turbulence and the laminar flame characteristics. In the Choi and Huh (1998) model (CH), $u'$ denotes the rms turbulent velocity and $l_c$ is an arbitrary length scale introduced for dimensional consistency and combined to $\alpha_0$ as a single arbitrary constant.
Figure 16: Experimental burner. A propane/air premixed flow is injected in a rectangular burner through a grid. The turbulent flame is stabilized behind a small cylinder (blockage ratio of 6%).

Figure 17: Transverse flame surface density ($\Sigma$) profiles ($m^{-1}$) plotted as a function of the transverse location for various downstream locations (mm downstream the rod). (a) $\phi = 0.78$; (b) $\phi = 0.9$. Flow rate: 35 g/s. From Veynante et al. (1996).
7.4.4 Comment: flame stabilization modeling

In Fig. 18 are compared the flame surface density fields obtained from laser tomography and the mean reaction rate estimated from CH radical emission. Close to the stabilization rod, the flame surface density $\Sigma$ is high whereas the mean reaction rate remains low. In fact, in this zone, fresh and burnt gases are separated by an interface (high surface densities) where combustion has started but is not yet established. This finding displays one of the difficulty of flame surface density models. In their present formulations, these models are unable to describe the flame stabilization because the $\Sigma$-equation (Eq. 6.3) is derived assuming that the flame does exist. All source terms in this equation are proportional to $\Sigma$ or to $\Sigma^2$ and the equation cannot generate flame surface when there is no initial flame surface. In addition, an initiation effect must also be incorporated to account for ignition time delay effects in the local reaction rate per unit surface, $Q_2$ (Eq. 6.2), to recover the observed results.
8 Turbulent transport in premixed combustion

8.1 Introduction

As described in section § 7, turbulent fluxes of the progress variable $c$, $\overline{\rho u''_i c''}$, is generally modeled using a classical gradient expression as for inert scalars:

$$\rho \overline{u''_i c''} = -\frac{\mu_t}{Sc_i} \left( \frac{\partial \overline{c}}{\partial x_i} \right)$$  \hspace{1cm} (8.1)

where $\mu_t$ is the turbulent viscosity estimated from the turbulence model and $Sc_i$ is a turbulent Schmidt number. Nevertheless, theoretical (Libby and Bray 1981) and experimental studies (Bray et al. 1981; Shepherd et al. 1982) have evidenced in some turbulent premixed flames counter-gradient turbulent transport where the turbulent fluxes $\overline{\rho u''_i c''}$ and the mean progress variable $\overline{c}$ gradient, $\partial \overline{c}/\partial x_i$, have the same sign in some regions and cannot be described with Eq. (8.1).

This quite surprising finding may be easily explained from the Bray-Moss-Libby analysis developed in section § 7.3. In this formulation, the turbulent fluxes of the progress variable $c$ are indirectly connected to fresh ($\overline{u''_i}$) and burnt gases ($\overline{u''_b}$) conditional velocities (Eq. 7.34, § 7.3.4):

$$\overline{\rho u''_i c''} = \overline{\rho c (1-c)} (\overline{u''_i} - \overline{u''_b})$$  \hspace{1cm} (8.2)

Even conditional velocities are not obvious quantities, this expression may be used to simply explain counter-gradient turbulent transport. Because of the thermal expansion due to combustion heat release, the burnt gases conditional velocity, $\overline{u''_b}$, is probably greater than the fresh gases conditional velocity, $\overline{u''_i}$. Accordingly, the turbulent fluxes of the progress variable $c$ have the same sign than the mean gradient $(\partial \overline{c}/\partial x_i)$, in opposition with model expression (Eq. 8.1).

This phenomenon is known as counter-gradient turbulent transport or counter-gradient turbulent diffusion. Counter-gradient transport is also found to increase when the heat release factor $\tau$, defined by Eq. (7.14), increases (Masuya and Libby 1981).

Counter-gradient turbulent transport has been evidenced by the derivation of the BML model (§ 7.3). In fact, the various versions of this BML model propose an algebraic closure for the mean reaction rate of the progress variable $c$ but focus the attention on the scalar turbulent transport description (closure schemes for the turbulent fluxes $\overline{\rho u''_i c''}$ balance equations) whereas other models may lead to more sophisticated reaction rate formulations, but retain a simple gradient closure (Eq. 8.1) for turbulent fluxes.

Recent studies based on direct numerical simulations of turbulent premixed flames without (Veynante et al. 1997) and with (Veynante and Poinset 1997a) externally imposed pressure gradients have confirmed that counter-gradient diffusion was found in simulations, but that classical gradient diffusion was also possible. A criterion to delineate between gradient and counter-gradient diffusion situations was derived from these studies, showing that counter-gradient may occur in practical situations. Counter-gradient transport is also analyzed in terms of
coherent structure motions in Veynante et al. (1996). Without any externally imposed pressure gradient, counter-gradient turbulent diffusion has to be expected when the Bray number \( N_B \) is higher than unity:

\[
N_B = \frac{\tau}{2\alpha \frac{u'}{S_L}} \leq 1 \tag{8.3}
\]

where \( \tau \) is the heat release factor \( (\tau = T_b/T_u - 1) \) where \( T_u \) and \( T_b \) are respectively the temperature of fresh and burnt gases and \( u'/S_L \) the velocity ratio between the RMS velocity \( u' \) and the laminar flame speed \( S_L \). \( \alpha \) is an efficiency function taking into account the fact that smaller turbulent length scales are unable to affect the flame front. \( \alpha \) is of order unity for large values of the length scale ratio \( t_L/\delta_L \) and decreases towards 0 for low length scale ratios (Veynante et al. 1997). The above criterion (Eq. 8.3) is displayed on Fig. 10 for \( \tau = 6 \). Counter-gradient turbulent transport is promoted by high values of the heat release factor \( \tau \) and by favorable externally imposed pressure gradients (i.e. pressure decreasing from fresh gases to burnt gases) (Veynante and Poinset 1997a) whereas high turbulence levels and adverse pressure gradients promote classical gradient turbulent diffusion.

Turbulent transport plays an important role in the propagation of turbulent premixed flames (Duclos et al. 1993). Accordingly, a more refined description of the turbulent fluxes (Eq. 8.1) is required. It is generally based on the closure of exact balance equations for \( \overline{\rho u'' Y_k''} \) (Bray et al. 1981; Bray et al. 1987; Bray 1987). Few attempts of such an approach are up to now available in practical situations (Bailly 1996; Bailly et al. 1996).
<table>
<thead>
<tr>
<th>Zone</th>
<th>$\bar{u}^i - \bar{u}^f$</th>
<th>$\frac{\partial \bar{c}}{\partial x}$</th>
<th>$\bar{w}'' c''$ (when $y &gt; 0$)</th>
<th>$\bar{v}^i - \bar{v}^f$</th>
<th>$\frac{\partial \bar{c}}{\partial y}$ (when $y &gt; 0$)</th>
<th>$\bar{w}'' c''$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$&lt; 0$</td>
<td>$&gt; 0$</td>
<td>$G$</td>
<td>$&gt; 0$</td>
<td>$&lt; 0$</td>
<td>$G$</td>
</tr>
<tr>
<td>2</td>
<td>$&gt; 0$</td>
<td>$&gt; 0$</td>
<td>$CG$</td>
<td>$&gt; 0$</td>
<td>$&lt; 0$</td>
<td>$G$</td>
</tr>
</tbody>
</table>

Table 2: Geometrical analysis of the scalar turbulent transport in a V-shape premixed flame (see Fig. 19). $G$ and $CG$ denote respectively a gradient and a counter-gradient turbulent diffusion.

8.2 Comment: an experimental result

Let us come back to the V-shape turbulent flame described in section § 7.4.3. The thermal expansion modifies the flame dynamics as clearly apparent on the high-speed tomography films (scheme in Fig. 19, Veyna et al. 1996): in the first part of the chamber (region 1), because of the rod wake, the coherent structures embedding the flame front turn from clockwise (counter-clockwise) in the upper (lower) flame sheet, as in classical Von Kármán vortex streets, except for their symmetry due to pressure waves. When the centerline velocity increases because of thermal expansion in burnt gases (region 2), the upper (lower) coherent structures start to turn counterclockwise (clockwise). This phenomenon may be recast in terms of turbulent transport using a simple geometrical analysis based on the Bray - Moss - Libby relation (8.2) and summarized in Table 2. Accordingly, transverse turbulent flux $\bar{v}'' c''$ is always of gradient type. But the change in structures rotation corresponds to a transition between gradient and counter-gradient transport for the downstream turbulent flux $\bar{v}'' c''$. The turbulent fluxes are of gradient type just behind the rod as expected to describe the flame stabilization and becomes of counter-gradient type further downstream.
9 Reynolds averaged models for nonpremixed turbulent combustion

Less attention has been focused on non-premixed turbulent combustion than on premixed turbulent combustion. In fact, in most practical situations, the reaction may be assumed to be very fast compared to mixing and diffusion times (large Damköhler numbers) corresponding to thin combustion layers ("flamelet"). Non-premixed combustion may also be described using passive scalar variables as previously described (see section 3.2). Accordingly, non-premixed turbulent combustion may be viewed as a mixing problem.

Models for non-premixed combustion are quite similar to those developed in the premixed case and differ only by their ingredients. These models may be summarized as follows:

9.0.1 Algebraic expressions

The Magnussen model, similar for non-premixed situations to the Eddy-Break-Up model, is the most popular algebraic model. The reaction rate is simply expressed as Magnussen and Mjertager (1976):

\[ \tilde{\omega}_F = \alpha \tilde{\theta} \frac{\varepsilon}{k} \min \left( \frac{\tilde{Y}_F}{s}, \frac{\tilde{Y}_O}{\gamma + s} , \beta \frac{\tilde{Y}_P}{1 + s} \right) \]  \hspace{1cm} (9.1)

where \( Y_F, Y_O \) and \( Y_P \) are respectively the fuel, oxidizer and product mass fractions. The parameter \( s \) is the mass stoichiometric coefficient of the chemical reaction Fuel \( \rightarrow \) Oxidizer \( \rightarrow \) Products, and \( \alpha \) and \( \beta \) are two model constants.

9.1 Flame surface density model

Flame surface density concepts have been firstly introduced by Marble and Broadwell (1977) to describe turbulent non-premixed combustion. The balance equation for the flame surface density \( \Sigma \) was based on phenomenological considerations starting from balance equation for a material surface where combustion effects have been intuitively added (Marble and Broadwell 1977; Fichot et al. 1994). Recent works (van Kalmthout et al. 1996; Van Kalmthout and Veynante 1997; Van Kalmthout and Veynante 1998) have provided an exact balance equation, identifying the flame surface to the stoichiometric iso-surface of the mixture fraction \( Z (Z = Z_{st}) \).

Let us point out that Fichot et al. (1994) have incorporated unsteady effects taking into account the flame time response on the local reaction rate per unit of flame area, following the analysis proposed by Haworth et al. (1988).

9.1.1 Probability density functions

This approach is similar to the one presented for premixed combustion. The probability density function is generally based on the passive scalar \( Z \) (see section 3.2) under the assumption of an
infinitely fast chemistry (Burke and Schumann limit) because mass fractions and temperature may be expressed as linear functions of \( Z \). In non-infinitely fast chemistry, the flow field is described with a PDF based on the passive scalar \( Z \) and the dissipation rate \( \chi \). Local mass fractions and temperature are then solutions of equations similar to Eq. (3.7). Assuming that the passive scalar \( Z \) and its dissipation are decoupled, the mean value \( \overline{Q} \) of any quantity \( Q \) is expressed as:

\[
\overline{Q} = \int_{\chi_1}^{\chi_2} \int_{0}^{1} Q(Z, \chi) p(\chi) d\chi dZ = \int_{\chi_1}^{\chi_2} \int_{0}^{1} Q(Z, \chi) p(Z) p(\chi) d\chi dZ
\]  \hspace{1cm} (9.2)

In the presumed probability framework, \( p(Z) \) is generally assumed to be a beta function whereas \( p(\chi) \) is modeled as a Gaussian function. The unclosed molecular diffusion term in the PDF balance equation (6.10) seems to be easier to model in non-premixed situations where the combustion rate is mainly controlled by molecular mixing.
10 Large eddy simulation

10.1 Introduction

Large eddy simulation (LES) is a very attractive tool for numerical simulations of fluid flows. The objective is to explicitly compute the largest structures of the flow field (typically the structures larger than the computational mesh size) whereas the effects of the small one are modeled. This technique is just at a very beginning stage for combustion modeling, (Veynante and Poinset 1997c) but a large amount of work has been conducted for non-reacting flow fields as evidenced in review papers by Piomelli and Chasnov (1996), Ferziger (1997), Lesieur (1997), Lesieur and Métais (1996).

Nevertheless, LES is a very promising approach for combusting studies:

- Large structures in a turbulent flows are generally assumed to depend on the system geometry whereas small structures have more universal features. Accordingly, models are probably more suited to describe these small structures.

- Most reacting flows exhibits large scale coherent structures. Such structures are also observed when combustion instabilities occur. These instabilities are due to a coupling between heat release, hydrodynamic flow field and acoustic waves. They have to be avoided because they induce noise, variations of the system characteristics, large heat transfers and may lead to the system destruction. LES could be a powerful tool to predict the occurrence of such instabilities (Menon and Jou 1991) and to numerically test passive or active control systems.

- The knowledge of large scale turbulent motions is very interesting to describe the effects of the unresolved smaller ones. In fact, subgrid scale models are generally based on similarity assumptions between large and small scales.

- Large eddy simulations could also allow a better description of the turbulence / combustion interactions because, in LES, large structures are explicitly computed and instantaneous fresh and burnt gases zones, where turbulence characteristics are quite different, are clearly identified.

In large eddy simulations, various quantities \( Q \) are filtered in the spectral space (components greater than a given cut-off frequency are suppressed) or in the physical space (weighted averaging in a given volume). The filtered quantity \( \overline{Q} \) is defined as:

\[
\overline{Q}(x) = \int Q(x') F(x - x') \, dx'
\]  

(10.1)

where \( F \) is the LES filter. In practical applications, the most popular filters are:
A cut-off filter in the spectral space:

$$F(k) = \begin{cases} 1 & \text{if } k \leq \pi/\Delta \\ 0 & \text{otherwise} \end{cases}$$

(10.2)

where $k$ is the spatial wave number. This filter keeps the length scales greater than the cut-off length scale $2\Delta$.

A box filter in the physical space:

$$F(x) = F(x_1, x_2, x_3) = \begin{cases} 1/\Delta^3 & \text{if } |x_i| \leq \Delta/2, i = 1, 2, 3 \\ 0 & \text{otherwise} \end{cases}$$

(10.3)

where $(x_1, x_2, x_3)$ are the spatial coordinates of the location $x$. This filter corresponds to an averaging of the quantity $Q$ over a box of size $\Delta$.

A Gaussian filter in the physical space:

$$F(x) = F(x_1, x_2, x_3) = \left(\frac{6}{\pi\Delta^3}\right)^{3/2} \exp\left[-\frac{6}{\Delta^2} \left(x_1^2 + x_2^2 + x_3^2\right)\right]$$

(10.4)

All these filters are normalized:

$$\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} F(x_1, x_2, x_3) \, dx_1 \, dx_2 \, dx_3 = 1$$

(10.5)

For variable density $\rho$, as in combusting flows, a mass-weighted, Favre filtering, is introduced according to:

$$\overline{\rho Q}(x) = \overline{\rho} \overline{Q}(x) = \int \rho(x') Q(x') \, F(x-x') \, dx'$$

(10.6)

Instantaneous balance equations (§ 2) are now filtered to derived balance equations for the filtered quantities $\overline{Q}$ or $\overline{\rho}$. But this derivation should be carefully conducted:

- Any quantity $Q$ may be split into a filtered component $\overline{Q}$ and a "fluctuating" component $Q'$, according to: $Q = \overline{Q} + Q'$. But, in disagreement with classical Reynolds averaging (ensemble average), $\overline{Q}'$ may be non zero:

$$\overline{Q}'(x) = \int (Q(x') - \overline{Q}(x')) \, F(x-x') \, dx'$$

$$= \int Q(x') \, F(x-x') \, dx' - \int \overline{Q}(x') \, F(x-x') \, dx'$$

$$= \overline{Q}(x) - \overline{Q}(x)$$

(10.7)
where
\[
\bar{Q}(x) = \int \left[ \int Q(x') F(x' - x'') dx'' \right] F(x - x') dx'
\]
\[= \int \int Q(x'') F(x' - x'') F(x - x') dx'' dx'
\]
\[\neq \bar{Q}(x) \tag{10.8}\]

To summarize:
\[
\bar{Q} \neq \bar{Q} ; \bar{Q}' \neq 0 ; \tilde{Q} \neq \bar{Q} ; \tilde{Q}' \neq 0 \tag{10.9}\]

Let us point out that relations \(\bar{Q} = \bar{Q}', \tilde{Q} = 0, \tilde{Q} = \bar{Q}, \tilde{Q}' = 0\) are true when a cut-off filter in the spectral space is used (Eq. 10.2). In this case, all the frequency components greater than a cut-off wavenumber \(k_c = \pi/\Delta\) are cancelled.

- The derivation of balance equations for the filtered quantities \(\bar{Q}\) or \(\tilde{Q}\) requires the exchange of filtering and derivation operators. This exchange is theoretically valid only under restrictive assumptions and is wrong, for example, when the filter size varies (filter size corresponding to the mesh size, depending on the spatial location). Ghosal and Moin (1995) have investigated this point in detail but, in general, the uncertainties due to this operator exchange is neglected and assumed to be incorporated in the subgrid scale models...

Large eddy simulations is also a challenge for experimentalists. Following the filtering operator previously described, simulated (filtered) or unresolved (subgrid scale) quantities, required to validate numerical simulations and improve modelling, have to be extracted from instantaneous 3D flow field imaging...

### 10.2 Filtered balance equations

Filtering the instantaneous balance equations leads to the following equations, formally similar to the Reynolds averaged balance equations displayed in Section 2.3:

- **mass**:
  \[
  \frac{\partial \bar{p}}{\partial t} + \frac{\partial \bar{p} \bar{u}_i}{\partial x_i} = 0 \tag{10.10}\]

- **momentum (for \(i = 1, 2, 3\))**:
  \[
  \frac{\partial \bar{p} \bar{u}_i}{\partial t} + \frac{\partial \bar{p} \bar{u}_j \bar{u}_i}{\partial x_j} = -\frac{\partial}{\partial x_i} \left[ \bar{p} (\bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j) \right] - \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \bar{F}_i \tag{10.11}\]
- **Chemical species** ($N$ species, $k = 1, \ldots, N$):
\[ \frac{\partial \bar{p} \bar{Y}_k}{\partial t} + \frac{\partial \bar{p} \bar{u}_j \bar{Y}_k}{\partial x_j} = -\frac{\partial}{\partial x_j} \left[ \bar{p} \left( u_j \bar{Y}_k - \bar{u}_j \bar{Y}_k \right) \right] + \bar{\omega}_k \]  
(10.12)

- **Total enthalpy** $h_t = h + u_i u_i/2$
\[ \frac{\partial \bar{p} \bar{h}_t}{\partial t} + \frac{\partial \bar{p} \bar{u}_j \bar{h}_t}{\partial x_j} = -\frac{\partial}{\partial x_j} \left[ \bar{p} \left( u_j \bar{h}_t - \bar{u}_j \bar{h}_t \right) \right] + \frac{\partial \bar{p}}{\partial t} + \frac{\partial}{\partial x_j} \left( \overline{\mathcal{J}_j^f + \bar{u}_i \bar{v}_j} \right) + u_j F_j \]  
(10.13)

where $\overline{Q}$ and $\bar{Q}$ denote LES filtered quantities and not ensemble means.

Unknown quantities must be modeled:

- **Unresolved Reynolds stresses** ($\bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j$), requiring a subgrid scale turbulence model.

- **Unresolved species fluxes** ($\bar{u}_i \bar{Y}_k - \bar{u}_i \bar{Y}_k$) and enthalpy fluxes ($\bar{u}_j \bar{h}_t - \bar{u}_j \bar{h}_t$).

- **Filtered laminar diffusion fluxes** $\overline{J}_j^f$, $\overline{J}_j^h$.

- **Filtered chemical reaction rate** $\bar{\omega}_k$.

These filtered balance equations, coupled to ad-hoc subgrid scale models may be numerically solved to extract the instantaneous filtered field. Compared to direct numerical simulations (DNS), the description of the unresolved small scales is lost. Compared to Reynolds ensemble averaging, large eddy simulations provide the instantaneous resolved field.

We will not provide here a description of the subgrid scale models for the unresolved turbulent fluxes because, as in RANS, reacting flows large eddy simulations use models developed for constant density flows. The reader may find more details in review papers by Piomelli and Chasnov (1996), Ferziger (1997), Lesieur (1997), Lesieur and Métai (1996). In the following, main LES combustion models are briefly described.

### 10.3 Simplest approaches for combustion modeling

#### 10.3.1 Arrhenius law based on filtered quantities

A first rough model is to neglect subgrid scale contributions and to write the reaction rate as an Arrhenius law for filtered quantities:
\[ \bar{\omega}_F = A \bar{p}^2 \bar{Y}_F \bar{Y}_O \exp \left( -\frac{E}{RT} \right) \]  
(10.14)

Such simplified expression assumes a perfect mixing at subgrid scale level (perfectly stirred reactor) and implicitly suppose that turbulent time scales, $\tau_t$, are shorter than chemical time.
scales $\tau_c$ ($\tau_t \ll \tau_c$). This assumption is generally used for reacting flows in atmospheric boundary layer (Nieuwstadt and Meeder 1997) but is clearly not relevant in most combustion applications.

A more refined approach is to take into account the segregation factor, as already described in RANS modeling (§ 4):

$$\Sigma_F = A \bar{\rho}^2 \bar{Y}_F \bar{Y}_O \exp \left( - \frac{E}{RT} \right) \left[ 1 + \frac{Y_F Y_O^m}{\bar{Y}_F \bar{Y}_O} \right]$$  \hspace{1cm} (10.15)

The segregation factor $I_{sgs} = Y_F^m / Y_F \bar{Y}_O$ is equal to 0 when the fuel and oxidizer are perfectly mixed at the subgrid level and $I_{sgs} = -1$ in a case of an infinitely fast reaction. $I_{sgs}$ may be presumed or found from a balance equation for $Y_F^m$ (Meeder and Nieuwstadt 1997). Once again, such an approximation is quite rough but may be justified when temperature fluctuations are negligible (for example for the dispersion of pollutants in the atmospheric boundary layer).

### 10.3.2 Extension of algebraic Favre averaged approaches

A simple idea is to extend Favre algebraic models such as Eddy-Break-Up model (§ 7.2) for premixed combustion or Magnusson model (§ 9.0.1) for non premixed combustion to LES (Fureby and Löfström 1994; Fureby and Möller 1995). For example, the subgrid scale Eddy-Break-Up model is simply written:

$$\bar{\omega}_F = C_{EBU} \bar{\rho} \frac{1}{\tau_t} \bar{Y}_F \left( 1 - \frac{\bar{Y}_F}{\bar{Y}_F} \right)$$  \hspace{1cm} (10.16)

where $\tau_t^{SGS}$ is a subgrid turbulent time scale, estimated as:

$$\tau_t^{SGS} = \frac{k^{SGS}}{\epsilon^{SGS}} \approx C_D \frac{\Delta \epsilon}{\sqrt{k^{SGS}}}$$  \hspace{1cm} (10.17)

where $k^{SGS}$ and $\epsilon^{SGS}$ are respectively the subgrid turbulent kinetic energy and its dissipation, $C_D$ a constant and $\Delta$ the filter size. The turbulent kinetic energy $k^{SGS}$ may be estimated from an algebraic model or a balance equation.

Such a simple formulation is quite attractive and has not been yet extensively tested. Nevertheless two drawbacks may be suspected. First, the Eddy-Break-up model has known deficiencies in Favre averaged context (reaction rate independent on chemical reaction, overestimation of the reaction rate in zones of strong shears...). In a LES context, the model constant $C_{EBU}$ seems to be strongly dependent on various parameters (flow conditions, mesh size,...).

### 10.4 LES models for non premixed combustion

As previously described (§ 5), in non premixed flames, turbulent times $\tau_t$ may often be assumed to be quite longer than characteristic chemical times $\tau_c$. Accordingly, such reacting flows are
Figure 20: "Triplet map" used in the Linear Eddy Model developed by Kerstein to simulate a one-dimensional turbulent stirring process. (a) before mixing; (b) simulated mixing by a vortex of size \( l \).

generally controlled by turbulent and molecular mixing processes. Two main ideas have been proposed to describe non-premixed combustion flow fields with LES: the Linear Eddy Model (LEM) mainly developed by Kerstein (Kerstein 1988; Kerstein 1989; Kerstein 1990; Kerstein 1991; Kerstein 1992) and the probability density function approach, initially proposed by Gao and O'Brien (1993) and developed further by various authors, such as Cook, Riley and their coworkers (Cook and Riley 1994; Cook and Riley 1998; De Bruyn Kops et al. 1998).

### 10.4.1 Linear Eddy Model

The Linear Eddy Model (LEM) developed by Kerstein (Kerstein 1988; Kerstein 1989; Kerstein 1990; Kerstein 1991; Kerstein 1992) is based on a one dimensional stochastic description of turbulent stirring processes. In a LES framework, this analysis is used to describe subgrid scale phenomena.

The turbulent stirring mechanism is modeled by a rearrangement process applied to the 1D scalar field. The initial scalar distribution (Fig. 20a) is rearranged on a given segment of size \( l \) according to Fig. 20b ("triplet map"). This process may be viewed as the effect of a single turbulent structure of size \( l \) located in \( x_0 \). Then, the turbulent mixing is simulated from a stochastic description where vortex locations \( x_0 \), vortex sizes \( l \) (\( l_k < l \leq \Delta \), where \( l_k \) is the Kolmogorov length scale and \( \Delta \) the LES filter size) and vortex frequencies \( \lambda \) are specified according to a given turbulence spectra (homogeneous turbulence in general).

**Molecular diffusion and chemical processes** are described by one dimensional balance equations:

\[
\frac{\partial \rho Y_i}{\partial t} = \frac{\partial}{\partial x} \left( \rho D_i \frac{\partial Y_i}{\partial x} \right) + \dot{\omega}_i \tag{10.18}
\]

To summarize, subgrid scale chemical reaction and turbulent mixing are analyzed from a one dimensional problem where a simple stochastic description of turbulence is achieved. Any complex chemistry or diffusion features may be easily incorporated in Eq. (10.18). This approach also provides a direct estimation of filtered mass fractions \( \overline{Y_i} \) or temperature \( \overline{T} \) without...
balance transport equations for these quantities. Nevertheless, mass fractions and temperature transports between adjacent mesh cells must be modeled. The LEM approach may also be quite time consuming because a one-dimensional calculation is required in each computational cell.

This approach is probably well suited for large eddy simulations of turbulent mixing (McMurthy et al. 1993) and non premixed combustion, at least when combustion phenomena are nearly mixing controled (McMurthy et al. 1992; Menon et al. 1994; Calhoun and Menon 1996; Mathey and Chollet 1997). But, despite some attempts (Menon and Kerstein 1992; Menon et al. 1993; Smith and Menon 1996), its extension to turbulent premixed combustion is more difficult. As pointed out by Poinset et al. (1991) and Roberts et al. (1993), viscous dissipation and flame front curvatures play an important role in flame / turbulence interactions and cannot be accounted for in LEM formulation.

### 10.4.2 Probability density functions

Under the assumption of fast chemistry, the species mass fractions \( Y_k \) and the temperature are functions of the passive scalar \( Z \) (see § 3). Then, the Favre filtered fuel mass fraction may be written as (Gao and O'Brien 1993):

\[
\tilde{Y}_f (x,t) = \frac{1}{\rho} \int_{-\infty}^{+\infty} \rho (x',t) Y_f (Z (x',t)) G (x - x') dx'
\]  

(10.19)

Introducing the Dirac \( \delta \)-function, expression (10.19) may be recast as:

\[
\tilde{Y}_f (x,t) = \frac{1}{\rho} \int_0^1 \int_{-\infty}^{+\infty} \rho (\Psi) Y_f (\Psi) \delta (Z (x',t) - \Psi) G (x - x') dx' d\Psi
\]  

(10.20)

leading to:

\[
\tilde{Y}_f (x,t) = \int_0^1 Y_f (\Psi) \frac{1}{\rho} \left[ \int_{-\infty}^{+\infty} \rho (\Psi) \delta (Z (x',t) - \Psi) G (x - x') dx' d\Psi \right] \text{ filtered PDF } \tilde{P} (\Psi, x, t)
\]  

(10.21)

Then:

\[
\tilde{Y}_f (x,t) = \int_0^1 Y_f (\Psi) \tilde{P} (\Psi, x, t) d\Psi
\]  

(10.22)

where the sub-grid probability density function \( \tilde{P} (\Psi, x, t) \) has been introduced. The problem is now to determine this probability density function. As for Favre averaged models (§ 6.2.1), this PDF may be either presumed or found from a transport equation.
**Presumed sub-grid PDF.** This approach has been firstly proposed, and tested against DNS and experimental data, for reacting flow by Cook and Riley (1994) for infinitely fast chemistry. For example, the filtered fuel mass fraction is given by:

\[
\tilde{Y}_f(x,t) = \int_0^1 Y_f(Z) \tilde{P}(Z, x, t) dZ
\]  

(10.23)

The authors have found that a \( \beta \) function (§ 6.2.1), based on the filtered passive scalar \( Z \) and its unresolved fluctuations \( \tilde{Z}^2 \) is very accurate. They also discussed a similarity model to describe the variance \( \tilde{Z}^2 \) without an additive balance equation:

\[
\tilde{Z}^2 = C_Z \left( \tilde{Z}^2 - \bar{Z}^2 \right)
\]  

(10.24)

where \( \tilde{Q} \) denotes a similarity filter. In recent works, Réveillon (1996), Réveillon and Veronis (1996), Réveillon and Veronis (1997) have proposed a dynamic procedure, similar to the Germano dynamic model to estimate \( C_Z \) leading to very promising results without solving a transport equation for the subgrid variance \( \tilde{Z}^2 \).

This approach has been extended to finite rate chemistry where the reaction depends on the mixture fraction \( Z \) and the scalar dissipation rate \( \chi_0 \) (see § 3.2.2) by Cook and Riley (1998, De Bruyn Kops et al. (1998):

\[
\tilde{Y}_f(x,t) = \int_0^1 \int_{\chi_0}^1 Y_f(Z, \chi_0) \tilde{P}(Z, \chi_0, x, t) d\chi_0 dZ
\]

\[
= \int_0^1 \int_{\chi_0}^1 Y_f(Z, \chi_0) \tilde{P}(Z, x, t) \tilde{P}(\chi_0, x, t) d\chi_0 dZ
\]  

(10.25)

where the joint pdf, \( \tilde{P}(Z, \chi_0, x, t) \) has been split into two independent pdfs. \( \tilde{P}(Z, x, t) \) is determined using a \( \beta \) function as described above. Chemistry features are incorporated from a counterflow strained flamelet assumption.

**Transport equation for the sub-grid PDF.** A transport equation for the subgrid scale PDF \( \tilde{P}(\Psi, x, t) \) may be derived (Gao and O'Brien 1993) and is formally similar to Eq. (6.10). This formalism has not yet been extensively tested (Réveillon and Veronis 1997).

**10.5 LES models for premixed combustion**

**10.5.1 Introduction**

A difficult problem is encountered for large eddy simulations of premixed flames: the thickness \( \delta_L \) of a premixed flame is about 0.1 to 1 mm and is generally smaller than the LES mesh size \( \Delta \) as plotted in Fig. 21. The progress variable (i.e. non dimensionalized fuel mass fraction or temperature) is a very stiff variable and the flame front cannot be resolved in the computation.
leading to numerical problems. To overcome this difficulty, two main approaches have been proposed: simulation of an artificially thickened flame or use of a flame front tracking technique (G-equation). A third one, based on the filtering of the \( r \) progress variable balance equation is developing.

### 10.5.2 Artificially thickened flames

The idea is to consider a flame thicker than the actual one, but having the same laminar flame speed \( S_L \) (Butler and O'Rourke 1977). Following simple theories of laminar premixed flame (Williams 1985; Kuo 1986), the flame speed \( S_L \) and the flame thickness \( \delta_L \) may be expressed as:

\[
S_L \propto \sqrt{aW} ; \quad \delta_L \propto \frac{a}{S_L}
\]
(10.26)

where \( a \) is the thermal diffusivity and \( W \) the mean reaction rate. Then, an increase of the flame thickness \( \delta_L \) by a factor \( \alpha \) with a constant flame speed \( S_L \) is easily achieved by replacing the thermal diffusivity \( a \) by \( \alpha a \) and the reaction rate \( W \) by \( W/\alpha \). If \( \alpha \) is sufficiently large (typically from 5 to 20), the thickened flame front may then be resolved on the LES computational mesh without subgrid modeling. The reaction rate is expressed using an Arrhenius law, as in direct numerical simulations.

This approach is very attractive:
• From a numerical point of view, the chemical reaction is described as in a direct numerical simulation on the LES computational grid, without subgrid scale model.

• Because of the use of an Arrhenius law, various phenomena are directly taken into account without requiring ad-hoc submodels (ignition, flame stabilization, flame/wall interactions...).

• Theoretically, this approach may be extended to complex chemistry.

This route has not been yet extensively tested in large eddy simulation (Thibaut and Candel 1998) but seems to be very promising, at least when the flow motions are far stronger than the laminar flame thickness, as in combustion instabilities (Veynante and Poinset 1997b).

Unfortunately, when the flame is thickened from $\delta_f$ to $\delta_f$, the interaction between turbulence and chemistry may be modified because the Damköhler number, $Da$, comparing turbulent ($\tau_t$) and chemical ($\tau_c$) time scales:

$$Da = \frac{\tau_t}{\tau_c} = \frac{l_p S_i}{u' \delta_f}$$

is decreased by a factor $\alpha$ and becomes $Da/\alpha$.

Accordingly, the interaction between flame and turbulence may be altered. Poinset et al. (1994) have shown that when the length scale ratio between the turbulent length scale and the laminar flame thickness, $l_p/\delta_f$, is decreased, the flame becomes more and more insensitive to turbulence motions. This ratio is decreased by a factor $\alpha$ when the flame is thickened. This point has been investigated using DNS by Angelberger et al. (1998) and an efficiency function $E$, depending on velocity ($u'/S_l$) and length scale ($\Delta/\delta_f$), has been derived to counteract this effect. In practical applications, the thickened flame approach is implemented by changing the diffusivity and the reaction rate according to (Angelberger et al. 1998):

Diffusivity: $a \rightarrow \alpha a$  
Reaction rate: $W \rightarrow W/\alpha \rightarrow EW/\alpha$

thickening  
wrinkling  

10.5.3 G-equation

In this approach, the flame surface is described as an infinitely thin propagating surface (flamelet). The key idea is to track the position of the flame front using a field variable $G$ (see § 6.1.1). The flame surface is associated to the isolevel $G = G^*$. The $G$-field does not have to follow the gradients of the progress variable $\epsilon$ and can be smoothed out to be resolved on the LES mesh. The $G$-equation is directly used for the resolved field $\overline{G}$, introducing a subgrid scale turbulent flame speed $\bar{S}_T$ (Kennard et al. 1988):

$$\frac{\partial \overline{G}}{\partial t} + \bar{u} \cdot \nabla \overline{G} = \bar{S}_T |\nabla \overline{G}|$$  

(10.28)
The challenge is then to propose a model for $\overline{S_T}$. This closure is generally based on Eq. (7.1):

$$
\frac{\overline{S_T}}{S_T} = 1 + \alpha \left( \frac{\overline{u^2}}{S_T} \right)^n
$$

(10.29)

where $\overline{u^2}$ is the subgrid scale turbulence level that may be estimated as:

$$
\overline{u^2} \approx \Delta \left[ \overline{S_T} \right] = \Delta \sqrt{\overline{S_{ij} S_{ij}}}
$$

(10.30)

where $S_{ij}$ are the components of the resolved shear stresses. The constants $\alpha$ and $n$ have to be specified. Im (1995) has proposed a dynamic determination for $\alpha$ when $n = 1$.

Equation (10.28) is a simple formulation corresponding to a simple physical analysis (displacement of the resolved flame front with the displacement speed $\overline{S_T}$). Nevertheless, as already pointed out (§ 7.1), the turbulent flame speed is not a well defined quantity and no universal model is available. Despite these drawbacks, the $G$-equation approach is, up to now, the most advanced technique for large eddy simulations of premixed combustion flow fields (Bourrioux et al. 1996; Menon 1996).

10.5.4 Filtering the progress variable balance equation

Assuming a single step chemistry and unity Lewis number (i.e. identical mass and thermal diffusivities), the mass fractions of the reactive species and the temperature are all linearly related and may be expressed in terms of a reaction progress variable $\gamma$ ($\gamma = 0$ within fresh reactants and $\gamma = 1$ within burnt products) as described in section 3.1, following the balance equation:

$$
\frac{\partial \rho \gamma}{\partial t} + \nabla \cdot (\rho \gamma \mathbf{u}) = \nabla \cdot (\rho D \nabla \gamma) + \mathbf{w} \cdot \nabla \rho \gamma = \rho \mathbf{w} \cdot \nabla \rho \gamma
$$

(10.31)

Applying the LES filter $F$, the previous $\gamma$-equation becomes:

$$
\frac{\partial \overline{\gamma}}{\partial t} + \nabla \cdot \left( \overline{\rho \mathbf{u} \gamma} \right) + \nabla \cdot [\overline{\rho (\mathbf{u} \gamma - \overline{\mathbf{u} \gamma})}] = \nabla \cdot (\overline{\rho D \nabla \gamma}) + \nabla \overline{\gamma}
$$

(10.32)

$$
= \overline{\rho \mathbf{w} \cdot \nabla \rho \gamma}
$$

(10.33)

where the three LES terms in Eq. (10.32) correspond respectively to unsteady effects, resolved convective fluxes and unresolved transport. The two RHS terms in Eq. (10.32) denote respectively filtered molecular diffusion and filtered reaction rate. The RHS term in Eq. (10.33) corresponds to flame front displacement.

As already pointed out, the flame front (and the gradient of the progress variable $\gamma$) is generally too thin to be resolved on the LES computational mesh. Nevertheless, following Bogor et al. (1998), the filtered progress variable $\overline{\gamma}$ may be resolved using a physical space Gaussian filter $F$ (Eq. 10.4) with a filter size $\Delta$ larger than the computational mesh size $\Delta_m$. points.
The $\bar{c}$-balance equation (10.33) is similar to a $C$-equation but, compared to an arbitrary $C$-field, the progress variable $c$ has a main advantage: $c$ and related quantities ($\Sigma^*, \Sigma, \langle pw \rangle, \ldots$) are physically defined and may be extracted from DNS or experimental measurements.

Boger et al. (1998) then propose a flame surface density formulation for subgrid scale modeling. The flame front displacement may be recast as (Piana et al. 1997):

$$\bar{pw} | \nabla \bar{c} | = \langle pw \rangle \Sigma = \langle pw \rangle \Xi | \nabla \bar{c} | \quad (10.34)$$

where $\Sigma$, $\langle Q \rangle$, and $\Xi$ represent, respectively subgrid scale flame surface density, surface average and subgrid scale flame surface wrinkling (i.e. subgrid flame surface divided by its projection in the propagating direction).

This approach is formally the same than the one derived for RANS in section 6.1.2. In fact, ensemble averages and surface averages are just replaced by filtered quantities.

$\langle pw \rangle$ and $\Xi$ now have to be modeled. In a first step, the surface-averaged mass-weighted displacement speed $\langle pw \rangle$ may be estimated from the laminar flame speed $S_L$ and the fresh gases density $\rho_o$ as:

$$\langle pw \rangle \approx \rho_o S_L \quad (10.35)$$

For example, subgrid scale flame surface densities $\Sigma$ and flame wrinkling factor $\Xi$ may be extracted from experiments (Boger and Veynante 1998) or direct numerical simulation data (Boger et al. 1998).

As in RANS, the flame surface density $\Sigma$ and the flame front wrinkling $\Xi$ may be expressed from:

- **Algebraic expressions.** Based, for example, on a BML-type approach (Boger et al. 1998):

$$\Sigma = 4 \sqrt{\frac{6}{\pi}} \frac{\varepsilon (1 - \varepsilon)}{\Delta} \quad (10.36)$$

where the subgrid scale flame wrinkling factor, $\Xi$ may be estimated from subgrid scale rms velocity, $u'_A$, as:

$$\Xi = 1 + \frac{u'_A^2}{S_L} \quad (10.37)$$

but more sophisticated expressions may be proposed (Angelberger et al. 1998). Flame surface densities may also be estimated from a fractal analysis. Dynamic formulations could be derived.

- **Balance equations.**

Starting from Eq. (10.31) and using previous definitions, there is no difficulty to derive exact, but unclosed, balance equations for $\Sigma$ (Boger et al. 1998). In fact, this equation is
formally identical to the balance equation for flame surface density (Eq. 6.3) widely used in Reynolds-averaged context (Trouvé and Poinset 1994; Vervisch et al. 1995). Weller et al. (1998) have closed and used a balance equation for the subgrid scale flame surface wrinkling factor, \( \Xi \), in LES.

The unresolved turbulent fluxes, \( \overline{\nu c} - \overline{\nu \overline{c}} \) remain to be modeled. Boulet et al. (1998) have found, analyzing DNS, that the unresolved transport exhibits gradient or counter-gradient features depending on the turbulence level and the heat release factor \( r \) as already observed in RANS (see § 8). Nevertheless, compared to RANS, unresolved fluxes are lower and, accordingly, model uncertainties will have less dramatic consequences in LES than in RANS.

To our mind, flame surface density analysis is more promising than the simple use of a subgrid turbulent flame speed \( \overline{S_T} \) in a \( \dot{c} \)-equation (Eq. 10.28). In its simplest form, this approach is similar but may be easily refined taking benefits of the various studies conducted in a RANS context (§ 7.4).

10.6 Numerical costs

Large eddy simulations are a very promising tool for turbulent combustion and combustion instabilities. But such simulations have a numerical cost that may becomes prohibitive:

- LES are, by definition, unsteady simulations. Accordingly, some usual assumptions used in computation of averaged flows cannot be retained (symmetry, two-dimensional mean flows, ...). A relevant description of the turbulent motions requires tri-dimensional simulations ...

- The mesh size (i.e. the filter size) should be sufficiently small. Most models derived to describe the unresolved fluxes are based on similarity assumptions requiring that the cut-off scale between resolved and unresolved structures is in the inertial range of the turbulence spectrum. Accordingly, a given range of turbulence motions has to be resolved.

- The numerical precision of the code is a key point: as more precise phenomena are described, compared to RANS simulations (subgrid fluxes), the subgrid scale models have not to be blur by the code numerical diffusion ...

- Initial and boundary conditions may be not obvious. For example, the numerical simulation of a turbulent flow in a channel requires to impose at the inlet an ad-hoc unsteady turbulent flow field. In non-reacting flows, numerical simulations generally assumed a periodic channel. With chemical reaction, or in a non-periodic configuration (obstacle, for example), a second simulation of a periodic channel may be used to provide the required instantaneous flow field ...
- Relevant averaged and global quantities (mean, rms, correlation functions, energy spectra,...) may be extracted from large eddy simulations but require a long computational time and large databases.

Accordingly, LES developments have to be conducted together with numerical (algorithm precision,...) and computational (code vectorization and parallelism) studies. For example, it remains unclear today whether "industrial" codes (KIVA, FLUENT...), suited to complex flow geometries, may be used for large eddy simulations...
11 CONCLUSIONS

Modeling and simulations of turbulent combustion is a difficult challenge. In combusting flow fields, various difficulties (strong heat release, large range of time and length scales,...) are added to the complexity of constant-density turbulent flows.

A summary of the most classical Reynolds (or Favre) averaged Navier-Stokes (RANS) description has been proposed. In such analysis, three main elements have to be modeled:

- Reynolds stresses $\overline{u_i u_j} - \overline{u_i u_j}$.

- Turbulent transport of species mass fractions $\overline{u_i Y_k} - \overline{u_i Y_k}$.

- Mean reaction rate $\overline{\omega_k}$.

Most works in turbulent combustion modeling have been devoted to propose refined descriptions for the mean reaction rate $\overline{\omega_k}$. Few studies have been done on species turbulent transport, generally modeled using a gradient expression whereas counter-gradient turbulent transport is known to occur in some situations. Reynolds stresses are generally described from classical turbulent models, simply re-written in terms of Favre averaged quantities. Combustion effects on the flow (flame induced turbulence generation, higher viscous dissipation ... ) are not explicitly taken into account.

Large eddy simulations is a very promising tool for combustion flow field description. First, such flows generally exhibit strong large scale coherent structures. LES could also provide a better description of turbulence / combustion interactions because fresh and burnt gases zones, having different turbulence characteristics, are instantaneously identified at the resolved grid level. Nevertheless, LES is only beginning for combustion applications and very few works have already been done on this subject, mainly devoted to feasibility tests (two dimensional simulations, constant density flows,...).
References


Combustion Systems and Modelling


the 8th Symposium (Int.) on Combustion, Naples. The Combustion Institute, Pittsburgh.


IMPROVEMENT OF THE MODELLING OF INDUSTRIAL FURNACES AND PROCESSES FOLLOWING EXPERIMENTAL OBSERVATIONS.

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ABSTRACT

Perlite rock is a volcanic mineral that can be expanded when heated rapidly at a temperature larger than 800 °C. The expanded material is then a very good thermal and sound insulating material. It can also be used in agriculture to retain water in the ground. For building and construction material applications, expanded perlite of uniform density and well-controlled size distribution is required. A computer code capable of predicting the combustion, the expansion process and the particle trajectories inside a vertical industrial furnace can serve in improving the quality of the final expanded product and in optimising the energy consumption inside the furnace by regulating the combustion parameters. In order to adopt the combustion code, measurements of temperature, velocity and concentrations of CO₂ have been performed. The improvement of the code will be presented.

This work has been performed at E.M2.C laboratory by K. Zähringer, J.-P. Martin, J.-P. Petit with the advice of N. Darabja and D. Veynaute. It has been supported in part by a European Union grant within the BRITE-EURAM program.

In the industrial process, perlite granulates (0.2 to 3 mm in size) are injected by gravity into a high vertical furnace. A large burner, located at the base of the furnace, producing a vertical flame heats the gases in the furnace. The perlite granulates fall into the flame, are heated by heat convection from the hot burning gases and by radiative transfer from the surrounding gas or by the hot walls of the furnace. When the perlite reaches a sufficient temperature, the glass soften, steam bubbles form in the particulate and the granulate expands (usually the volume of the particulate is multiplied by 10). The expanded perlite is blown up by the flow and is evacuated at the top of the furnace. Figures 1 and 2 show a side and top view of the trajectories of particulate through the furnace. The different trajectories are caused by the turbulence of the flow.

We have developed a numerical simulation of the combustion, the mechanical interaction of the perlite with the turbulent flow, for the heat transfer to the particulate and the expansion phenomenon (Klipfel 1999). We have used the k-ε model for turbulence, a unique chemistry reaction (fuel + air → H₂O + CO₂) and the conventional Eddy Brake Up (EBU) model is used to calculate the local reaction rate. In order to test the results of the code and also to have reliable values for the description of the initial flow field in the burner and the furnace, we have performed measurements:
- Temperature field at three locations across the furnace with conventional thermocouples equipped with an anti radiative screen,
- Velocity measurement with a Pitot tube in the flame and with a hot wire at the exit of the burner before ignition,
- Temperature of the furnace walls with an optical pyrometer,
- Temperature of the particulate and the soot (if present) in the furnace.

It is worth to note that the furnace was equipped with only one thermocouple placed in the flue gases at the exit of the furnace, and by two flow meters that deliver the flow rate of the air and fuel injected into the furnace.

The results of the velocity measurements at the exit of the burner are shown on figure 3 together with the data injected in the code. There exists a strong swirl at the exit of the burner.

A global check of the predicted temperature and speed at three locations in the furnace shows a good agreement between the measured and calculated values (figure 4).

A more detailed (figure 5) comparison of the temperature field across the flame, show that the calculation predicts too high a temperature near the walls of the furnace. This is a usual behaviour of the EBU model, near walls it predicts too large reaction rate so that in these zones the predicted temperature is too high. We have modified the EBU model to take this problem into account and obtained the results shown on figure 6, the fit between the measured and calculated values is reasonable. The code has been used to predict the expansion of the perlite and give a good prediction of the quality of the expanded material. It has been used to improve the use of the furnace in order to produce new products.

As the code has proved to predict properly the production of perlite in a vertical furnace, we used it to model the behaviour of a different furnace in which we performed similar measurements. Figure 7 presents the temperature profiles measured and calculated in the new furnace, the fit is not good and we are presently modifying the model.

This example has been given to show that:
1. conventional and low cost experimental techniques are still useful for industrial measurements
2. rather simple models can be used
3. these models have to be checked and must be adapted to a given situation.

Trajectories of non-isothermal particles,
d=1 mm, improved model

Laboratoire E.M2.C.
Trajectories of non-isothermal particles,
Furnace cross section, d=1 mm, improved model
Comparaison : écoulement gazeux

Mesures

850°C
30 m/s

1000-1200°C
25 m/s

paroi:
750-800°C

1000-1100°C
20 m/s

4-7 m/s

paroi:
800-900°C

1000-1050°C
17 m/s

condition d’entrée

Laboratoire E.M2.C
FIGURE 5: Measured and calculated temperature across the furnace (original EHU)
FIGURE 6: Measured and calculated temperature (ESU modified)
FIGURE 7: Measured and calculated temperature across the furnace.

- \( \text{temperature at } x = 0.461 \text{m} \)
- \( \text{temperature at } x = 1.91 \text{m} \)
- \( \text{temperature at } x = 3.33 \text{m} \)

- \( \text{v \text{-values calculated}} \)
- \( \text{v \text{-values measured A}} \)
- \( \text{v \text{-values measured B}} \)
MONITORING PROCESSES
MONITORING PROCESSES

MONITORING AIR POLLUTANTS IN COMBUSTION

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ABSTRACT

An attempt is being made to explore possible sources of emissions from the operation of Combustion Systems (mobile and stationary sources) and the need to use laser to monitor the emission gases and other pollutants from the activities of some industries in Ghana.

1.0 INTRODUCTION

1.1 COMBUSTION SYSTEMS

Combustion systems can be derived generally from both internal combustion engines and external combustion sources. Internal combustion engines may be stationary and mobile in nature. Major items within stationary combustion engines category are gas turbines and large heavy duty general utility reciprocating engines. Most stationary internal combustion engines are used to generate electric power, to pump gas or other fluids or to compress air for pneumatic machinery. Stationary gas turbines find its application in electric power generators, in gas pipelines pump and compressor drives, in various process industries. Gas turbines emit considerably smaller amounts of pollutants than do reciprocating engines; however, reciprocating engines are generally more efficient in their use of fuel. Reciprocating which may be 2-stroke lean burn, 4 stroke lean burn and 4-stroke rich burn affect some how both baseline emissions as well as the potential for emissions control.

Gasoline and Diesel industrial engines covers a wide variety of industrial applications such as aerial lifts, fork lifts, mobile refrigeration units, generators, industrial sweepers, material handling equipment and portable well drilling equipment.
1.2 EMISSIONS

The primary pollutants from internal combustion (IC) engines are oxides of nitrogen (NO\textsubscript{x}), organic compounds (hydrocarbons), carbon monoxide (CO), and particulates, which include both visible (smoke) and nonvisible emissions. Ash and metallic additives in the fuel also contribute to the particulate content of the exhaust. Oxides of sulphur (SO\textsubscript{x}) also appears in the exhaust from IC engines.

Pollutants of concern from large stationary diesel and all stationary dual fuel engines is NO\textsubscript{x}, which readily forms in the high temperature, pressure, nitrogen content of the fuel, and excess air environment found in these engines. Lesser amounts of CO and hydrocarbons are emitted. The sulphur compounds, mainly SO\textsubscript{2}, are directly related to the sulphur content of the fuel. SO\textsubscript{x} emissions will usually be quite low because of the negligible sulphur content of diesel fuels and natural gas.

1.3 CONTROLS

All reciprocating internal combustion (IC) engines operate by the same basic process. A combustible mixture is first compressed in a small volume between the head of a piston and its surrounding cylinder. The mixture is then ignited, and the resulting high pressure products of combustion push the piston through the cylinder. This movement is converted from linear to rotary motion by crankshaft. The piston returns, pushing out exhaust gases, and the cycle is repeated.

Moreover, large stationary diesel and all stationery dual fuel engines, supply mechanical power to operate drilling equipment and operate pumps. Smaller uses include irrigation and hoisting.

In all these examples, various measures are taken in the engine design and operations to minimise emission of pollutants. For instance, nitrogen oxide (NO\textsubscript{x}) emissions from regenerative cycle turbines are greater than emissions from simple cycle turbines because of the increased combustion air temperature entering the turbine. The carbon monoxide (CO) and hydrocarbon (HC) emissions may be lower with regenerative system for a comparable design. In addition, water/steam injection is the most prevalent (NO\textsubscript{x}) control for cogeneration/combined cycle gas turbines.

On the other hand, selective catalytic reduction (SCR) is a post-combustion control which selectively reduces NO\textsubscript{x} by reaction of ammonia and NO on a catalytic surface to form N\textsubscript{2}, H\textsubscript{2}, and O. Although (SCR) systems can be used alone, all existing applications of SCR have been used in conjunction with water/steam injection controls.

Table 1 and Table 2 give emission factors from both controlled and uncontrolled gas turbines and some trace elements. The major variables affecting NO\textsubscript{2} emissions from compressor engines include the air-fuel ratio, engine load, intake air temperature and absolute humidity. Table 3 shows some of the control technologies that indicate possible parameters which can reduce or increase the diesel emissions.
**TABLE 1  TRACE ELEMENT EMISSION FACTORS FOR DISTILLATE OIL-FIRED GAS TURBINES**

*(Emission Factor Rating E)*

<table>
<thead>
<tr>
<th>Trace Element</th>
<th>Pg/J</th>
<th>lb/MMBtu</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aluminium</td>
<td>64</td>
<td>5.5 E-04</td>
</tr>
<tr>
<td>Antimony</td>
<td>9.4</td>
<td>22 E-05</td>
</tr>
<tr>
<td>Arsenic</td>
<td>2.1</td>
<td>4.9 E-06</td>
</tr>
<tr>
<td>Barium</td>
<td>8.4</td>
<td>2.0 E-05</td>
</tr>
<tr>
<td>Beryllium</td>
<td>.14</td>
<td>3.3 E-07</td>
</tr>
<tr>
<td>Boron</td>
<td>28</td>
<td>6.5 E-05</td>
</tr>
<tr>
<td>Bromine</td>
<td>1.8</td>
<td>4.2 E-06</td>
</tr>
<tr>
<td>Cadmium</td>
<td>1.8</td>
<td>4.2 E-06</td>
</tr>
<tr>
<td>Calcium</td>
<td>330</td>
<td>7.7 E-04</td>
</tr>
<tr>
<td>Chromium</td>
<td>20</td>
<td>4.7 E-05</td>
</tr>
<tr>
<td>Cobalt</td>
<td>3.9</td>
<td>9.1 E-06</td>
</tr>
<tr>
<td>Copper</td>
<td>578</td>
<td>1.3 E-03</td>
</tr>
<tr>
<td>Iron</td>
<td>256</td>
<td>6.0 E-04</td>
</tr>
<tr>
<td>Lead</td>
<td>25</td>
<td>5.8 E-05</td>
</tr>
<tr>
<td>Magnesium</td>
<td>100</td>
<td>23 E-04</td>
</tr>
<tr>
<td>Manganese</td>
<td>145</td>
<td>3.4 E-04</td>
</tr>
<tr>
<td>Mercury</td>
<td>.39</td>
<td>9.1 E-07</td>
</tr>
<tr>
<td>Molybdenium</td>
<td>3.6</td>
<td>8.4 E-06</td>
</tr>
<tr>
<td>Nickel</td>
<td>526</td>
<td>1.2 E-03</td>
</tr>
<tr>
<td>Phosphorus</td>
<td>127</td>
<td>3.0 E-04</td>
</tr>
<tr>
<td>Potassium</td>
<td>185</td>
<td>4.3 E-04</td>
</tr>
<tr>
<td>Selenium</td>
<td>2.3</td>
<td>5.3 E-06</td>
</tr>
<tr>
<td>Silicon</td>
<td>575</td>
<td>1.3 E-03</td>
</tr>
<tr>
<td>Sodium</td>
<td>590</td>
<td>1.4 E-03</td>
</tr>
<tr>
<td>Tin</td>
<td>35</td>
<td>8.1 E-05</td>
</tr>
<tr>
<td>Vanadium</td>
<td>1.9</td>
<td>4.4 E-06</td>
</tr>
<tr>
<td>Zinc</td>
<td>294</td>
<td>6.8 E-04</td>
</tr>
</tbody>
</table>

a. Emission factor ratings of "E" indicate that the data are from a limited data set and may not be representative of a specific source or population of sources.
Table 2. (Metric Units) Emission Factors for Large Distillate Oil-Fired Controlled Gas Turbines\(^n\)

<table>
<thead>
<tr>
<th>Pollutant</th>
<th>Emission Factor</th>
<th>Emission Factor Rating</th>
<th>Water Injection (0.8 water/fuel ratio) (grams/kW-hr) a (power output)</th>
<th>(ng/J) (fuel input)</th>
</tr>
</thead>
<tbody>
<tr>
<td>NO</td>
<td>E</td>
<td></td>
<td>1.41</td>
<td>125</td>
</tr>
<tr>
<td>CO</td>
<td>E</td>
<td></td>
<td>0.090</td>
<td>8.26</td>
</tr>
<tr>
<td>TOC (as methane)</td>
<td>E</td>
<td></td>
<td>26</td>
<td>2.96</td>
</tr>
<tr>
<td>SO(^b)</td>
<td>E</td>
<td>b</td>
<td>b</td>
<td>b</td>
</tr>
<tr>
<td>PM</td>
<td>E</td>
<td></td>
<td>0.181</td>
<td>16.00</td>
</tr>
</tbody>
</table>

a. Calculate from fuel input assuming an average heat rate of 8,000 Btu/hp-hr (x3.632)
b. All sulphur in the fuel is assumed to be converted to SO\(_{x}\).

Table 3: Diesel Emission Control Technologies\(^n\)

<table>
<thead>
<tr>
<th>Technology</th>
<th>Affected Parameter Increase</th>
<th>Decrease</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel Modifications</td>
<td>PM, Wear, PM, NO(_{x})</td>
<td>PM, NO(_{x})</td>
</tr>
<tr>
<td>Sulphur Content Increase</td>
<td>PM, NO(_{x})</td>
<td>PM</td>
</tr>
<tr>
<td>Aromatic Content Increase</td>
<td>PM, NO(_{x})</td>
<td>PM</td>
</tr>
<tr>
<td>Cetane Number</td>
<td>PM, NO(_{x})</td>
<td>PM</td>
</tr>
<tr>
<td>10 percent and 90 percent Boiling Point</td>
<td>PM, NO(_{x})</td>
<td>PM</td>
</tr>
<tr>
<td>Fuel Additive</td>
<td>PM, NO(_{x})</td>
<td>PM</td>
</tr>
<tr>
<td>Water/Fuel Emulsion</td>
<td>PM, NO(_{x})</td>
<td>PM</td>
</tr>
<tr>
<td>Engine Modifications</td>
<td>NO, PM, BSFC, NO(_{x}), NO</td>
<td>NO, PM</td>
</tr>
<tr>
<td>Injection Timing</td>
<td>Power</td>
<td>NO, PM</td>
</tr>
<tr>
<td>Fuel Injection Pressure</td>
<td>NO, PM</td>
<td>NO</td>
</tr>
<tr>
<td>Injection Rate Control</td>
<td>NO, PM</td>
<td>NO</td>
</tr>
<tr>
<td>Rapid Spill Nozzles</td>
<td>NO, PM</td>
<td>NO</td>
</tr>
<tr>
<td>Electronic Timing &amp; Metering</td>
<td>NO, PM</td>
<td>NO</td>
</tr>
<tr>
<td>Injector Nozzle Geometry</td>
<td>NO, PM</td>
<td>NO</td>
</tr>
<tr>
<td>Combustion Chamber Modifications</td>
<td>NO, PM</td>
<td>NO</td>
</tr>
<tr>
<td>Turbocharging</td>
<td>PM, Power</td>
<td>NO</td>
</tr>
<tr>
<td>Charge Cooling</td>
<td>PM, Power</td>
<td>NO</td>
</tr>
<tr>
<td>Exhaust Gas Recirculation Oil</td>
<td>PM, Power, Wear</td>
<td>NO</td>
</tr>
<tr>
<td>Consumption Control</td>
<td>PM, Power, Wear</td>
<td>NO</td>
</tr>
<tr>
<td>Exhaust After Treatment</td>
<td>PM, Wear</td>
<td>NO</td>
</tr>
<tr>
<td>Particulate Traps</td>
<td>NO</td>
<td>NO</td>
</tr>
<tr>
<td>Selective Catalytic Reduction</td>
<td>NO</td>
<td>NO</td>
</tr>
<tr>
<td>Oxidation Catalysts</td>
<td>NO</td>
<td>NO</td>
</tr>
<tr>
<td>NO(_{x}) = Nitrogen oxides; PM = Particulate matter; HC = Hydrocarbons; CO = Carbon monoxide; BSFC = Brake specific fuel consumption</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Combustion, Diagnostics and Optical Techniques 124
1.4 Emission Dynamics

Gaseous emissions from combustion processes is derived from Oxides of sulphur (Sulphur dioxide, sulphur trioxide), Carbon monoxide particulate (dust, smoke, fly ash, mist), hydrocarbons (hexane, benzene, methane butane etc.) oxides of Nitrogen and hydrogen fluoride.

Nitrogen oxides (NO_x) emissions can be formed from these processes such as

\[
\begin{align*}
N_2 + O_2 & \rightarrow 2NO \\
N_2 + 2O_2 & \rightarrow 2NO_2
\end{align*}
\]

About 90 to 95% of NO and 5 to 10% of NO_2 are found in the flue gas. NO_x formation results from fuel bound Nitrogen and Nitrogen in combustion air. On the other hand NO_x combustion controls tend to depend on air-fuel ratio. Efforts to reduce in NO_x emissions results in increase in carbon monoxide and unburned hydrocarbon emissions.

The essence in reducing NO_x emissions tend to be advantageous as an ozone and acid rains precursor. However, optimised combustions operations help to minimize CO and UHC emissions. Loss on ignition and very low operation cost. In addition, the use of oxidation catalysts assist to limit CO and VOC emissions. Such catalysts may be precious metal (Platinum). Post Combustion NO_x emissions control has been found effective using selective catalysts and selective Non-catalytic reduction.

2.0 MONITORING TECHNIQUES

Monitoring of Combustion systems is essential since

i. it is required by regulation to know actual pollution levels,
ii. it provides accurate emission data
iii. it provides data input for modelling and predictions
iv. it provides information about plant performance as well as optimising operations of other combustion systems.

The basic means of monitoring is the continuous emissions monitoring equipment (CEM) that can be mounted on all new electric generation stations, and in some cases, retrofit monitoring on existing stations. CEM has been found useful since it can monitor flow gas such as:

- CO_2 - 13%, N_2 - 76%, O_2 - 7%, NO_X - 9 to 500 ppm
- SO_2 - 30 to 1800 ppm, SO_3 - 0.1 to 20 ppm
- Ash - 0.0040 to 4 grains and ml/standard m^3
- HCl - 0 to 100 ppm

There are three basic techniques used in continuous emission monitoring (CEM) which are

i. absorption spectroscopy,
ii. luminescence spectroscopy and
iii. electro-analytical methods. [4]
Methods (i) and (ii) could be applied by using laser as a source depending on the wavelength.

2.1 ABSORPTION SPECTROSCOPY

Absorption spectroscopy which makes use of scattering of incident light by solids or gases is used to determine spectra of the absorbed lines of the species. Analysis of such operations depend heavily on the Beer-Lambert's Law which states that the absorbance $A$ is proportional to the concentration of absorbers in the sample which is expressed as:

$$ A = \ln \frac{1}{T} = \alpha \cdot c \cdot l \quad (1) $$

where $T$ is the transmittance and is the ratio of the intensity of the light passing through the sample $P_i$ to the intensity of the light entering the sample $P_0$. $\alpha$ is the attenuation coefficient of pollutant $c$ is the concentration of pollutant and $l$ is the distance the light beam travels through the flame.

The relative accuracy in the concentration determination is given by

$$ \frac{\Delta C}{C} = \frac{\Delta A}{A} \quad (2) $$

Analysis by optical techniques has found the use of relation between absorption and concentration quite useful. This principle is quite useful for monitoring opacity and for some gas monitoring techniques [5]. Opacity uses the laser techniques to measure blockage of visible image because of plume. The principle relies on scattered particulate and its size and concentration measurement. It is observed that less light leaves than enters and it is related to path length. It has a correlation possible for specific fuel and combustor as well. Opacity monitoring can be a single pass or double pass as shown in Fig 1. Measurement made, can be evaluated using the expression:

$$ \text{Opacity at stack exit} = 1 - \left(1 - \text{opacity at monitor location}\right)^a $$

where

$$ a = \frac{\text{stack exit path length}}{\text{monitor path length}} $$

These analysers cannot be zeroed using the same light source with the generating unit on-line. Either a second light or some other method must be used for zero calibration.

The differential absorption analysis technique compares an absorbed wavelength of light to a non-absorbed wavelength of light to determine gas concentrations. Differential absorption is used for NO and SO$_2$ measurements based on non-dispersive ultraviolet and for CO$_2$ and H$_2$O measurements based on non-dispersive infrared. The single beam dual wavelength analysis technique uses narrow-band optical filters to select infrared wavelengths. The second derivative spectroscopy uses ultraviolet light to measure SO$_2$ and NO concentrations, and its based on the varying spectral absorption of gas molecules. The set up are shown in Fig 1 - 3.
The general technique of differential absorption uses two different wavelengths of incident light. One wavelength is selected to be absorbed by the pollutant of interest. The other wavelength, a reference wavelength, should be absorbed by the pollutant of interest but should be very close to the measurement wavelength. Such a system can be modified by using a tunable laser to explore the range.

2.2 FLUORESCENCE

Fluorescence techniques use light to excite the gas molecules so that the difference in the wavelength of the exciting light and the emitted light can be determined. Fluorescence is used to determine the SO$_2$ concentration. It however interferes with H$_2$ ornamentation, CO$_2$ and O$_3$ which are manifested as a quenching of the emitted light. To eliminate the interference, the calibration gas must contain the interference in the same concentration as exist in the gas stream being analysed. Using Laser technique ensure that an atom state is to detect the fluorescence light released when the atom decays. The atom can return to the state from which it was excited via an allowed electric dipole transition. Flame Photometry is a technique that excites the gas sample to luminescence by introduction into a flame. The flame generally used is fueled by hydrogen. The spectra given off by the host gases are analyzed in the ranges of interest. This technique is sensitive to sulphur. Flame photometry is very effective for ambient level monitoring.

Other in situ monitor systems may be across-the-stack and point type. Across-the-stack analysers are single pass because of the limited transmission of the ultraviolet and infrared wavelengths. These analysers cannot be used if there is significant particulate concentration or uncombined water droplets. Single point in situ analysers make their measurements over a very short path length, usually a few cm. These analysers can function in high dust concentrations and situations where there are water droplets because the measurements cavity is protected by a ceramic filter. Laser technique has an advantage of using lidar to monitor inaccessible points.
(a) Single pass Transmissometer

(b) Double Pass Transmissometer

Figure 1: Opacity Monitor Systems[4]
Figure 2: In Situ Differential Absorption Analyzer [4]
Figure 3: Second Derivative Spectroscopy Analyser [4]
MONITORING GASES AS Emitted FROM THE STACK

Fig 4: Optical System for monitoring gases from the initial stages of Combustion System in high stacks at in using monochromator.
Light Scattering System for remote sensing.
MONITORING SITUATION

Monitoring as gases are emitted into Atmosphere

Fig. 6a

Ejected Gases in Atmosphere

LIDAR

Pol.

Fig. 6b
3.0 INSTRUMENTATION

Other commercial instruments such as Laser dust monitor (of sensidyne, inc.) determines relative concentrations of airborne dust passing a laser light source. The scattered light produces an electrical signal and the dust concentration is instantly displayed in counts per minute (CPM) with a sensitivity as low as 0.001 mg/M³. This value can be correlated to the mass concentration of a particular type of dust by multiplying by the “K” factor conversion coefficient for the particular dust. This K factor for any dust may be determined by a one time simultaneous comparison to a gravimetric sample. A continuous emission monitoring device SM8100A which permits in situ gas measurements without any sample preparation measure the narrowband absorption of ultraviolet radiation that is characteristics or specific to SO₂ and NO molecules. The SM8100A can be combined with an opacity monitor, an oxygen or CO/CO₂ analyser and the controller. A combination system provides continuous output for opacity, pollutant concentrations, excess air levels, temperature, total emission rates and parts per million (ppm). Most of the traditional instruments for monitoring gaseous particulates (SO₂, NOx and CO₂) are Dust reading meters while the VOC's make use of Gas chromatography. In addition air borne particulate matter are measured with PM10 and PM 2.5 respectively while Heavy and Trace elements are also measured with X-ray Fluorescence and Reactor Neutron Activation Analysis (RNA)AA.

4.0 LASER OPTION

The Laser option makes use of all the emission monitoring techniques which include absorption and emission spectroscopy and image processing. [6] The techniques apply to both light absorption, Fluorescence and light scattering that are sensitive to concentration and path length of the pollutants.

Fig. 4 makes use of an optical system using light scattering at the initial stages of the stack of the oil refinery or from the aluminium smelter. and Fig 5 makes use of remote sensing and absorption technique as the signal is directed into the monochromator for analysis.

Fig. 6, shows how laser light when shot into the atmosphere scatter the pollutants and receives the backscatter for analysis. All these examples give effective means of monitoring emission of gases from combustion systems which can be applied to most industries in Ghana.

5.0 Ghana Situation

In Ghana, a number of human activities give rise to pollutants. The major activities in this category are transportation (vehicular), fuel combustion for stationary sources (thermal plant). Industrial processes, solid waste disposal and burning wild forest fires (agricultural) give a lot of major emissions. Most of the equipment used for particulates, oxides of sulphur, nitrogen and carbon and hydrocarbons are gravimetric, calorimetric, reflectometric and CO meters used along major vehicle routes in the cities. The point source of emission of these pollutants from the Tema Oil Refinery may be many meters above the ground or not easily accessible for the use of the traditional monitoring equipments already listed. Some of the emissions guidelines from EPA is shown at Table 4.
<table>
<thead>
<tr>
<th>SUBSTANCE</th>
<th>TIME WEIGHT AVERAGE (TWA) WEIGHTED</th>
<th>AVERAGE TIME</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sulphur Dioxide (SO₂)</td>
<td>Industrial 900µg/m³</td>
<td>1 hr.</td>
</tr>
<tr>
<td></td>
<td>Residential 700µg/m³</td>
<td>1 hr.</td>
</tr>
<tr>
<td></td>
<td>Industrial 150µg/m³</td>
<td>24 hrs</td>
</tr>
<tr>
<td></td>
<td>Residential 100µg/m³</td>
<td>24 hrs</td>
</tr>
<tr>
<td></td>
<td>Industrial 80µg/m³</td>
<td>1 hr.</td>
</tr>
<tr>
<td></td>
<td>Residential 400µg/m³</td>
<td>1 hr.</td>
</tr>
<tr>
<td></td>
<td>Industrial 150µg/m³</td>
<td>1 hr.</td>
</tr>
<tr>
<td></td>
<td>Residential 60µg/m³</td>
<td>24 hrs</td>
</tr>
<tr>
<td>Nitrogen Oxides (measured as NO₂)</td>
<td>Industrial 230µg/m³</td>
<td>24 hrs</td>
</tr>
<tr>
<td></td>
<td>Residential 150µg/m³</td>
<td>24 hrs</td>
</tr>
<tr>
<td></td>
<td>Industrial 75µg/m³</td>
<td>1 yr</td>
</tr>
<tr>
<td></td>
<td>Residential 60µg/m³</td>
<td>24 hrs</td>
</tr>
<tr>
<td>Total Suspended Particulate (TSP/SPM)</td>
<td>Residential 70µg/m³</td>
<td>1 yr</td>
</tr>
<tr>
<td></td>
<td>Industrial 150µg/m³</td>
<td>24 hrs</td>
</tr>
<tr>
<td></td>
<td>Residential 100µg/m³</td>
<td>24 hrs</td>
</tr>
<tr>
<td></td>
<td>Industrial 50µg/m³</td>
<td>1 yr</td>
</tr>
<tr>
<td></td>
<td>Residential 30µg/m³</td>
<td>15 mins</td>
</tr>
<tr>
<td></td>
<td>Industrial 100µg/m³</td>
<td>30 mins</td>
</tr>
<tr>
<td></td>
<td>Residential 60µg/m³</td>
<td>1 hr</td>
</tr>
<tr>
<td></td>
<td>Industrial 30µg/m³</td>
<td>8 hrs</td>
</tr>
<tr>
<td></td>
<td>Residential 10µg/m³</td>
<td></td>
</tr>
<tr>
<td>PM10 Smoke</td>
<td>Residential</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Industrial</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Residential</td>
<td></td>
</tr>
<tr>
<td>Carbon Monoxide (CO)</td>
<td>Residential</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Industrial</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Residential</td>
<td></td>
</tr>
</tbody>
</table>

Subject to further studies

Hydrogen Fluoride and NOx from Volta Aluminium Company (VALCO) are also emitted from an alumina smelting stack over 30m in height. All these sources are not easily accessible. Gases such as CO₂, N₂, SO₂ are emitted at the mines at Nsuta and Tarkwa. Goldmines in Bogoso, Prestea, Obuasi and others tend to emit gases from the sulphur material that is roasted into oxide by combustion process. Pioneer Tobacco Company and Cocoa Processing Company at Takoradi use boilers and give scanty emissions of CO, NO₂ O₂. Monitoring has not been very
effective as there has been short fall in the monitoring equipment. As a result, there are no numerical data and environment related information. Through the Environmental Protection Agency, EPA, has guidelines for emissions in the country are available but there is lack of equipment to do such effective monitoring at the industrial cities and the mining towns to know actual emission levels. There is the need to look for equipment to do effective on line monitoring using the laser technique. The laser systems ensure real-time, fast, non-perturbing monitoring. In addition there is no need to transport sample and could use wide bandwidth since there are tunable sources. It is therefore essential to make use of DOAS and DIAL Laser systems to have effective monitoring.

6.0 CONCLUSION

Optical methods of monitoring Combustion processes have been found useful by looking at its merits from the advanced discussion. However, there is no effective means of measurement due to lack of equipment, personnel and support. This paper is suggesting that the Regional Laser Centre should be used for on job training in combustion diagnostics in combustion diagnostics of up coming scientists. Coordinated team of the research institutions, industries and the Universities are needed to explore emission areas and to help solve some of the problems at hand. It is realised that the Laser system could be a better option to make valuable contribution to the data required for decision making.
REFERENCES


[6] Sune Svanberg, “Atomic and Molecular spectroscopy – Basic Aspects and Practical Applications” 2nd Ed. Springer Verlag, Berlin Chapt. 9 and 10 (pp. 235-341)
FIGURE CAPTIONS

Fig 1: Opacity monitor systems  
   a. Single pass transmissometer 
   b. Double Pass transmissometer 

Fig. 2. In situ Differential Absorption Analyser. 

Fig. 3. Second derivative spectroscopy Analyser. 

Fig. 4. Optical system for monitoring gases from the initial stages of combustion in high stacks using monochromator. 

Fig. 5. Light Scattering System for monitoring gas emission in remote atmosphere using automated spectrometer. 

Fig. 6.  
   a) Monitoring gases emitted into the atmosphere through the exit of the stack. 
   b) Emitted gases into the atmosphere are back scattered for detection using LIDAR.
NEEDS FOR OPTICAL MEASUREMENTS IN COMBUSTION PROCESSES FOR ENERGY EFFICIENCY IMPROVEMENT AND POLLUTION ABATEMENTS

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ABSTRACT

The detailed modelling of combustion processes and of industrial furnaces is not yet by the numerical tools presently available: the models do not contain all the physical and chemical information needed for a correct modelling. Moreover, even if these knowledge were available the computing power of the machines and the computing time necessary to solve the problems would not be reasonable. Thus approximations and simplifications need to be done so that results must be validated nearly for each application. In a large number of cases, the model itself has to be adjusted for each application in "real life". The test must be done by measuring different key parameters (temperature, velocity field, molecular concentrations, $\mathcal{S}$). In parallel to mechanical traditional techniques which are intrusive, optical non-intrusive techniques can be used. These techniques give access to temperature, molecular or radical concentrations, velocity and can give local information, follow time evolutions of the parameters, or global or averaged values. Some of the techniques will be presented.

1.0 INTRODUCTION

Measuring different key parameters (temperature, velocity field, and molecular concentrations...) must do the test. In parallel to mechanical traditional techniques that are intrusive, optical non-intrusive techniques can be used. These techniques give access to temperature, molecular or radical concentrations, and velocity and can give local information, follow time evolutions of the parameters and global or averaged values.

When developing a measuring protocol, we have first to ask, and answer the two questions: why do I want to measure? And generally the answer to the next question: what to measure? is straightforward.

Combustion is the main source of energy for industrial (and household) processes; it will remain so for a long time, so it is of a major interest for economical and social aspects. As it has been described in other lectures, combustion is unfortunately the source of pollutants such as CO, NOx, SOx, HF, ozone, PAH, soot particulate...Generally when a combustion process emits large quantities of pollutants it also shows a poor energy efficiency. Energy saving and pollutant abatement are generally linked. The solutions to these problems needs technical studies which, as
higher constraints are applied, are not sufficient to solve the problem. New knowledge is needed and scientific research has to be developed in order to acquire improved physical and chemical models, which in turn are, includes in numerical modelling.

The chemical reactions (when known) take place (see Veynante) in turbulent or laminar flows, the reactants are either premixed or diffuse in each other, before or during reaction, the fluids can be in the gas phase or, in part, solid or liquid (two phase combustion). The description of the flow (especially turbulent flows) and its coupling with the chemical reactions relies on models which are based on several assumptions, thus the results of any modelling has to be validated and the range and cases for which it is reliable has to be determined. This is the role of diagnostics, which has to deal with the flow field, temperature, stable molecules and radical concentration. We have to measure either local values or its field repartition; time averaged or its evolution with time.

2.0 Some examples:

2.1 Evolution of the OH LIF signal in a counter flow diffusion flame.

We have developed (Rolon, 1991) a burner that is producing a laminar flat diffusion flame. This burner can be operated between atmospheric pressure up to 30 bar. The flame is perfectly known, extensive and detailed measurements as well as numerical prediction can be performed. OH can be used to trace the flame location, we performed OH Laser Induced Fluorescence (LIF) measurements at different pressure. Figure 1 shows the evolution of the LIF signal at 1, 2 and 4 bar. At 1 bar, the LIF signal is unique, at 2 bar a second zone, situated above the flame location (which is visualised by the more intense signal) appears. For 4 bar the lower signal is more intense than the top one. Calculations and a more detailed analysis show that the lower signals at 2 and 4 bar are the LIF signal generated by soot precursors; the fuel is heated before reaching the flame front and PAH are generated.

2.2 Interaction of a vortex with a flat flame.

The burner producing the flat diffusion laminar flame has been modified to study the interaction of a single ring vortex in the fuel flow. This vortex travels through the fuel flow and interacts with the flat flame. Figure 2 show an OH LIF visualisation of the time evolution of the flame when it is modified by the vortex crossing the reaction (flame) zone. The more intense flame zones are visualised by the brighter zone in the image. One can see that the flame intensity (burning rate) is higher in some zone and that it can be reduced in other places. in some places the flame can be extinguished. This illustrates the influence of the stress imposed by the flow to the flame. The information contain in these pictures are used in developing fundamental turbulent flame models.

2.3 Pollutant (NOx and CO) formation in a water heater gas appliance.

CO and NOx emissions are usually produced in flame when the reactions take place within some temperature ranges. An illustration of the evolution of CO and of NOx in a gas appliance, are shown on figure 3 (Coghi, 1995). It can be shown that when the emission of CO is reduced it can be followed by the increase in the emission of NOx. This behaviour is general, and some techniques for reducing the emissions have been developed. It consists in using totally
premixed lean combustors. For the most developed realisations the combustion take place in two stages, one lean combustion at low temperature avoids the formation of NOx, a second rich zone is used to burn the formed CO into CO₂. The overall pollution is reduced. Unfortunately this solution can lead to combustion instabilities and the burner can emit noise.

### 2.4 Interaction of a plane acoustic wave with a laminar premixed flame.

Turbulent flames generate noise, it has been shown that pressure fluctuation generated by the noise can modify the flame behaviour; and in certain cases can lead to dramatic flame extinction. We have designed an experimental set-up (associated to a computer modelling) to study the interaction of a premixed laminar flame with a superimposed sinusoidal plane acoustic wave. Figure 4 shows the flame before the acoustic wave is applied and when the wave is applied. The flame front is visualised by four-colour strioscopy. The flame surface adapts to the pressure modification and the overall burning rate is, in that case, increased.

### 2.5 Examples for the set of chemical reactions to be included in detailed chemistry combustion modelling.

The cruder combustion models include only one total chemical reaction in the description of the flame. For example methane flame are described by:

\[ \text{CH}_4 + 2 \text{O}_2 \rightarrow \text{CO}_2 + 2 \text{H}_2\text{O} + \text{energy} \]

Table 1 shows some of the 284 chemical reactions that can be necessary to model the combustion of CH₄ in air especially when pollutants formation has to be calculated. In most of the models, and especially in turbulent combustion, it is impossible to include the complete set of reactions in the model. Reduced chemistry (usually 2 to 3 reactions) has to be used and assumption on the importance of the different chemical paths for the reaction has to be adopted. Katta (1998) shows the results of such assumptions on the prediction of different species in a CH₄ – air flame (figure 5). Well chosen measurements have to be developed in order to test the results of the code.

### 2.6 Validity of a modelling for different test cases.

We have developed a model (Rolon, 1994) to calculate OH and temperature fields in our laminar counter flow diffusion flame. It has been used for the prediction of the behaviour of CH₄ – air, C₃H₈ – air, and H₂ – air flames. We also measured temperature field by Rayleigh scattering and OH by Laser Induced fluorescence. On figures 6 to 8 we compare the measured and calculated values. For CH₄ and C₃H₈ the model reproduces nearly perfectly the measured values. Thus both the experimental measurement technique and computer model are validated. For the hydrogen-air flame a systematic difference is shown. Further modelling showed that the diffusion rate of hydrogen in air is not correctly predicted in such flames.
REFERENCES:
Experiment in fluids 1991, 11, 313

J.-C. Rolon, N. Darabiha, T. Croonenbroek, T. Dagusé.

A; Coghi, G. Zizak, G. Solero, E. Sebastiani, M. Geghi.
Conference “Combustion technology for a clean environment”, Lisbon 1995

Figure 1: LIF imaging of OH radical in a flat counterflow diffusion CH₄ – air flame at different pressure. The flame position is indicated by the OH LIF signal. For \( p = 4 \) bar the sensitivity for the camera was reduced to avoid saturation of the pixels, OH LIF signal is in fact stronger than for 2 bar.
Figure 2: OH LIF during the interaction between a ring vortex and a flat counterflow diffusion CH$_4$ - air flame.
Figure 3: NOx and CO emissions as a function of the CO₂ percentage in the flue gases
Figure 4: Interaction between a laminar CH4 - air premixed flame and a plane acoustic wave
Figure 5: Results of a modelling of a CH₄ – air flame with different reduced chemistry schemes.
Counterflow diffusion flame CH₄ - air at atmospheric pressure

(\(\phi = 3.5\); \(v_{\text{air}} = 0.8\) m/s; \(v_{\text{fuel}} = 0.8\) m/s; \(\varepsilon = 106\) s\(^{-1}\))

**OH concentration**
- LIF
- theory

**Temperature:**
- Rayleigh
- theory

OH concentration (molecules/cm\(^3\) / 10\(^16\))

Position on z axis [mm]

Temperature [K]

Air \(\rightarrow\) CH₄ + N\(_2\) \(\rightarrow\)
Counterflow diffusion flame $C_2H_4$ - air at atmospheric pressure

$\phi = 3.5, v_{air} = 0.8 \text{m/s}, v_{fuel} = 0.8 \text{m/s}, e = 1.06 \text{s}$

Rayleigh - theory

$C_3H_8 + N_2$

Air

$OH$ concentration

$OH$ concentration

$\text{OH concentration (molecules/cm}^3\text{)}$
Counterflow diffusion flame $\text{H}_2$-air at atmospheric pressure

$(\phi = 1.0; v_{\text{air}} = 0.4 \text{m/s}; v_{\text{fuel}} = 0.4 \text{m/s}; \epsilon = 80 \text{ s}^{-1})$

**OH** concentration
- LIF
- theory

**Temperature**
- Rayleigh
- theory

[Graph showing OH concentration and temperature profiles along the z-axis for a counterflow diffusion flame of $\text{H}_2$-air at atmospheric pressure.]

Air $\rightarrow$ [Graph showing OH concentration and temperature profiles along the z-axis for a counterflow diffusion flame of $\text{H}_2$-air at atmospheric pressure.]

$\text{H}_2 + \text{N}_2$ $\rightarrow$ [Graph showing OH concentration and temperature profiles along the z-axis for a counterflow diffusion flame of $\text{H}_2$-air at atmospheric pressure.]

Position on z-axis [mm]
## Monitoring Processes

### Table 1: Some reaction to be taken into account for the modelling of a CH4 – air flame.

<table>
<thead>
<tr>
<th>No.</th>
<th>Reactions</th>
<th>No.</th>
<th>Reactions</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$\text{OH} + \text{O}_2$ → $\text{OH} + \text{O}$</td>
<td>254</td>
<td>$\text{NCO} + \text{M}$ → $\text{N} + \text{CO} + \text{M}$</td>
</tr>
<tr>
<td>2</td>
<td>$\text{O} + \text{H}_2$ → $\text{OH} + \text{H}$</td>
<td>255</td>
<td>$\text{NCO} + \text{H}$ → $\text{NH} + \text{CO}$</td>
</tr>
<tr>
<td>3</td>
<td>$\text{OH} + \text{H}_2$ → $\text{H}_2\text{O} + \text{H}$</td>
<td>256</td>
<td>$\text{NCO} + \text{O}$ → $\text{NO} + \text{CO}$</td>
</tr>
<tr>
<td>4</td>
<td>$\text{2OH}$ → $\text{H}_2\text{O} + \text{O}$</td>
<td>257</td>
<td>$\text{NCO} + \text{OH}$ → $\text{NO} + \text{CHO}$</td>
</tr>
<tr>
<td>5</td>
<td>$\text{O}_2 + \text{H} + \text{M}$ → $\text{HO}_2 + \text{M}$</td>
<td>258</td>
<td>$\text{NCO} + \text{NO}$ → $\text{N}_2 + \text{CO}_2$</td>
</tr>
<tr>
<td>6</td>
<td>$\text{H}_2\text{O}_2 + \text{H}$ → $\text{H}_2 + \text{O}_2$</td>
<td>259</td>
<td>$\text{NCO} + \text{N}$ → $\text{N}_2 + \text{CO}$</td>
</tr>
<tr>
<td>7</td>
<td>$\text{H}_2\text{O}_2 + \text{H}$ → $\text{H}_2 + \text{O}_2$</td>
<td>260</td>
<td>$\text{NCO} + \text{NO}$ → $\text{H}_{2}\text{CO} + \text{NO}$</td>
</tr>
<tr>
<td>8</td>
<td>$\text{H}_2\text{O}_2 + \text{H}$ → $\text{H}_2 + \text{O}_2$</td>
<td>261</td>
<td>$\text{NCO} + \text{CO}_2$ → $\text{N}_2 + \text{CO} + \text{CO}$</td>
</tr>
<tr>
<td>9</td>
<td>$\text{H}_2\text{O}_2 + \text{H}$ → $\text{H}_2 + \text{O}_2$</td>
<td>262</td>
<td>$\text{NCO} + \text{CO}_2$ → $\text{N}_2 + \text{CO} + \text{CO}$</td>
</tr>
<tr>
<td>10</td>
<td>$\text{H}_2\text{O}_2 + \text{H}$ → $\text{H}_2 + \text{O}_2$</td>
<td>263</td>
<td>$\text{NCO} + \text{O}_2$ → $\text{NO} + \text{CO}_2$</td>
</tr>
<tr>
<td>11</td>
<td>$\text{2H} + \text{M}$ → $\text{H}_2 + \text{M}$</td>
<td>264</td>
<td>$\text{HNCO} + \text{M}$ → $\text{NCO} + \text{H} + \text{M}$</td>
</tr>
<tr>
<td>12</td>
<td>$\text{2H} + \text{H}_2\text{O}$ → $\text{H}_2 + \text{H}_2\text{O}$</td>
<td>265</td>
<td>$\text{NCO} + \text{H}_2$ → $\text{HNCO} + \text{H}$</td>
</tr>
<tr>
<td>13</td>
<td>$\text{2H} + \text{H}_2\text{O}$ → $\text{H}_2 + \text{H}_2\text{O}$</td>
<td>266</td>
<td>$\text{HNCO} + \text{H}<em>2$ → $\text{N}</em>{2}\text{O} + \text{CO}$</td>
</tr>
<tr>
<td>14</td>
<td>$\text{2H} + \text{CO}_2$ → $\text{H}_2 + \text{CO}_2$</td>
<td>267</td>
<td>$\text{HNCO} + \text{O}$ → $\text{NO} + \text{CO}$</td>
</tr>
<tr>
<td>15</td>
<td>$\text{H} + \text{OH} + \text{M}$ → $\text{H}_2\text{O} + \text{M}$</td>
<td>268</td>
<td>$\text{HNCO} + \text{O}$ → $\text{NO} + \text{CO}$</td>
</tr>
<tr>
<td>16</td>
<td>$\text{2O} + \text{M}$ → $\text{O}_2 + \text{M}$</td>
<td>269</td>
<td>$\text{HNCO} + \text{O}$ → $\text{NO} + \text{CO}$</td>
</tr>
<tr>
<td>17</td>
<td>$\text{CO} + \text{OH}$ → $\text{CO}_2 + \text{H}$</td>
<td>270</td>
<td>$\text{HNCO} + \text{OH}$ → $\text{NO} + \text{H}_2\text{O}$</td>
</tr>
<tr>
<td>18</td>
<td>$\text{CO} + \text{HO}_2$ → $\text{CO}_2 + \text{OH}$</td>
<td>271</td>
<td>$\text{HNCO} + \text{OH}$ → $\text{NO} + \text{H}_2\text{O}$</td>
</tr>
<tr>
<td>19</td>
<td>$\text{CO} + \text{O} + \text{M}$ → $\text{CO}_2 + \text{M}$</td>
<td>272</td>
<td>$\text{HNCO} + \text{ON}$ → $\text{HCON} + \text{NO}$</td>
</tr>
<tr>
<td>20</td>
<td>$\text{CO} + \text{O}_2$ → $\text{CO}_2 + \text{O}$</td>
<td>273</td>
<td>$\text{HNCO} + \text{NH}$ → $\text{NH}_2 + \text{HCON}$</td>
</tr>
<tr>
<td>21</td>
<td>$\text{CH} + \text{OH}$ → $\text{CHO} + \text{H}$</td>
<td>274</td>
<td>$\text{HNCO} + \text{H}$ → $\text{CN} + \text{H}_2\text{O}$</td>
</tr>
<tr>
<td>22</td>
<td>$\text{CH} + \text{CO}_2$ → $\text{CHO} + \text{CO}$</td>
<td>275</td>
<td>$\text{HNCO} + \text{H}$ → $\text{NCO} + \text{H}_2$</td>
</tr>
<tr>
<td>23</td>
<td>$\text{CH} + \text{O}$ → $\text{CO} + \text{H}$</td>
<td>276</td>
<td>$\text{HNCO} + \text{OH}$ → $\text{NCO} + \text{H}_2\text{O}$</td>
</tr>
<tr>
<td>24</td>
<td>$\text{CH} + \text{OH}$ → $\text{CHO} + \text{H}$</td>
<td>277</td>
<td>$\text{HNCO} + \text{O}$ → $\text{NO} + \text{OH}$</td>
</tr>
<tr>
<td>25</td>
<td>$\text{OH} + \text{H}_2\text{O}$ → $\text{CH}_2\text{O} + \text{H}$</td>
<td>278</td>
<td>$\text{H} + \text{CH}_3$ → $\text{CH}_2\text{O} + \text{H}$</td>
</tr>
<tr>
<td>26</td>
<td>$\text{OH} + \text{H}_2\text{O}$ → $\text{CH}_2\text{O} + \text{H}$</td>
<td>279</td>
<td>$\text{NO} + \text{CH}_3$ → $\text{HCON} + \text{OH}$</td>
</tr>
<tr>
<td>27</td>
<td>$\text{CH}_3 + \text{CO}_2$ → $\text{CH}_2\text{O} + \text{H}$</td>
<td>280</td>
<td>$\text{NH} + \text{H}_2\text{O}$ → $\text{HCON} + \text{OH}$</td>
</tr>
<tr>
<td>28</td>
<td>$\text{CH}_3 + \text{CO}_2$ → $\text{CH}_2\text{O} + \text{H}$</td>
<td>281</td>
<td>$\text{H}_2\text{CN} + \text{H}$ → $\text{HCON} + \text{H}_2$</td>
</tr>
<tr>
<td>29</td>
<td>$\text{CH}_3 + \text{CO}_2$ → $\text{CH}_2\text{O} + \text{H}$</td>
<td>282</td>
<td>$\text{H}_2\text{CN} + \text{OH}$ → $\text{HCON} + \text{H}_2\text{O}$</td>
</tr>
<tr>
<td>30</td>
<td>$\text{CH}_3 + \text{CO}_2$ → $\text{CH}_2\text{O} + \text{H}$</td>
<td>283</td>
<td>$\text{H}_2\text{CN} + \text{M}$ → $\text{HCON} + \text{H} + \text{M}$</td>
</tr>
<tr>
<td>31</td>
<td>$\text{CH}_3 + \text{CO}_2$ → $\text{CH}_2\text{O} + \text{H}$</td>
<td>284</td>
<td>$\text{H}_2\text{CN} + \text{H}_2$ → $\text{CH}_2(\text{CO}) + \text{H}_2$</td>
</tr>
</tbody>
</table>
AETHALOMETER APPLICATIONS FOR REAL-TIME MONITORING OF COMBUSTION-DERIVED AEROSOL CARBON

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Obafemi Awolowo University, Ile-Ife, Nigeria.

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4905 Dufferin Street, Downsview Ontario 5T4
Canada.

ABSTRACT

The paper reviews the combustion process, the formation of elemental carbon and its potential usefulness as a tracer for combustion of carbonaceous fuels. It further reviews the literature on the methods available for the measurement of elemental carbon and discusses in detail the aethalometer, an instrument for real-time measurement of elemental (black) carbon developed at the Lawrence Berkeley Laboratory, USA. The physical configuration details and the datalogger programmes written by the authors for its field use are presented. Typical data obtained from a major field testing of the instrument are presented.

1.0 Literature Survey on Methods of Measurement of Elemental Carbon

Elemental carbon is an ubiquitous, strongly optically absorbing aerosol species resulting from the combustion of carbonaceous fuels. It comprises a graphitic microcrystalline structure (Rosen et al. 1978, Novakov (1984), Wolff (1984)).

Besides its importance as a contributor to visibility extinction in the urban atmosphere, it is also a very useful tracer of anthropogenic activity, almost in the same way that condensation nuclei is an indicator of aerosols. Also, because it is essentially non-reactive, it is conserved during long range transport, it is often measured at remote locations in order to unravel the sources of any air pollution found threat.

Elemental carbon can generally be measured in one of the following ways: (a) optical techniques such as Raman spectroscopy, infra-red absorbance or visible light absorbance measurements, the integrated plate method (Sadler et. al. (1981)) and the aethalometer, (b) photoacoustic techniques (Szkalat and Japar (1983)). (c) thermal methods such as temperature-programmed pyrolysis (Cachier et. al. (1989)) or stepwise pyrolysis and oxidation (Cadle and Groblicki (1982)) and (d) combined optical/thermal technique such as was used by Huntzicker et. al. (1982). The major setback of the thermal analysis of elemental carbon is the pyrolytic conversion (charing) of organic carbon to soot carbon which confounds the results. The optical techniques do not have such a drawback but are themselves sensitive to the loading of the collection filter surface as well to the morphology of the aerosol particles (Cadle and Groblicki (1982)). All the above methods with
the exception of the aethalometer involve grab sampling and, of necessity, a time-lag before the carbon concentration is determined. By contrast, the aethalometer combines the elegance of the optical technique with the possibility of real time measurement. Such real time measurements facilitate plume studies as well as the measurement of the atmospheric vertical profiles from aircraft-mounted aethalometers in major global atmospheric chemistry studies.

The theoretical basis for the design of the aethalometer has been reported by Rosen et al, 1978, Rosen et al, 1980, Hansen et al, 1982 and Gundel et al 1984. But, the Atmospheric Environment Service Laboratory at Downsvie was among the first to subject the instrument to an independent testing outside the laboratory where it was developed. The experience gained in that regard forms the basis for this paper.

2.0 The Aethalometer

(a) Principle of operation

The aethalometer (see Fig 1) measures the absorbance of elemental particles and converts these into voltage which are amplified in a photomultiplier. The flow of sample is constrained to the centre of the filter paper by means of a seal 'O' ring (the "signal voltage" refers to this core). The outer perimeter of the paper is retained as clean and provides the "reference voltage". After a predetermined interval, the measurements of signal and reference voltage are made with the instrument light on (for \(R_L\) and \(S_L\) voltages) and with the light off (for \(R_D\) and \(S_D\) voltages). These values are combined with the values at the end of the preceding interval to compute the elemental carbon concentration. The effective mean reference and signal voltage during the interval can be obtained as:

\[
R = R_L - R_D \\
S = S_L - S_D
\]
FIG. 1A: SCHEMATIC DIAGRAM OF THE AETHALOMETER (SIDE VIEW)

AA - AETHALOMETER HEAD PIECE
AB - AETHALOMETER BASE
AC - CLAMPING HO
AD - FILTER PAPER
AE - SEAL "O"-RING
AF - TEST-LAMP
AG - SAMPLED AIR INLET
AH - SAMPLED AIR OUTLET (CONNECTED TO PUMPING UNIT INLET)
AJ - SPRIN

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Fig. 2
The voltages over two consecutive intervals are used for the computation of concentration in the following manner.

\[
\text{EC Conc} = -100 \times 10000 \times \frac{\ln (S/R)_{t+1} - \ln (S/R)_t}{\text{SA} \times \text{FL} \times t}
\]

(1)

where

\[
\begin{align*}
\text{MA} & = \text{filter mask area, cm}^2 \\
\text{SA} & = \text{specific attenuation cross section for elemental carbon on quartz fibre filter} \\
& \quad \text{\hspace{1cm} (= 25 m}^2\text{g}^{-1}) \\
\text{FL} & = \text{flow rate through the filter, litres per minute} \\
\text{t} & = \text{time interval (minutes)}
\end{align*}
\]

b) **Physical configuration**

The physical configuration is depicted in Fig 2. The measurement principles is based on the circuitry represented in Fig 3. The field experience of the authors was that the instrument was sensitive to high frequency electromagnetic radiation. The ground of the first version had to be adjusted in order to reduce the instrument "noise" that plagued that version. Thereafter, the instruments performed very beautifully.

3.0 **Programming for field application**

The CR21X datalogger programme comprised the following segments: (a) setting the ports and sampling intervals, (b) activating the relays to control (on an on/off basis) the aethalometer lamp and sampling pump flow (c) reading the ports at present intervals, (d) calculation of concentrations from the voltage measurements and (e) setting flags on basis of loading of the filter. The flow chart that was adopted is presented as Fig 4. Important fragments of the programme are provided as Appendix B. The detailed programme listing is available on request. The possibility of remote access to the programme and data were built into the programme. The aethalometers were prepared for installation at the BAPMON uploaded and results downloaded via E.O.S. (an older version of internet) to the computers at the Atmospheric Environment Service laboratory, Downsview, Ontario.

4.0 **Intercomparison of the aethalometer output with an independent optical analysis.**

Five exposed filters were sent to an independent laboratory for measurement of the black carbon loading by means of an independent optical analysis method. The results were compared with the integrated black carbon concentration based on the aethalometer measurements. The comparison is presented in Table 1.

5.0 **Measurement of detection limits**

The detection limits of the aethalometer was determined by running the instrument on a clean air source. The clean air was obtained by inserting a high efficiency, two stages, quartz filter paper on the inlet of the aethalometer. The use of bottled zero air was not favoured for reasons of cost. The standard deviation of the voltages measured over 48 hours were used in calculating the error of the elemental carbon concentrations that would be evaluated from the voltage measurements as shown in Appendix A. The measured voltages and their standard deviation are presented in Table 2.
Initialize locations, battery voltage display, low pass filter, set resolution to high, active storage area P2, P30, P58, P80

If $T=0$ (i.e. top of the hour)

- Yes → Set Output Flag = 0
- No → Set resolution to High, set active storage area, calculate averages, maximum, minimum, Std.dev. of parameters, set real time P78, P80, P71, P77, P70, P73, P74, P82

If $51 < T < 60$

- Yes
- No
Read voltages and store in designated memory space P31

CALL SUBROUTINE 2 P86

Set Relay Port to "High" (to switch on aethalometer lamp)
If \( T = 60 \)

Yes

Set Hour counter, Record SIGNAL & REFERENCE voltages P32, P31

CALL SUBROUTINE 3

Reset Relay Port to "Low" Calculate voltage differences P20, P35.
If \( T = 60 \)

Yes

Set Resolution to "High", Set Real time on

If Output Flag = 0

No

CONTINUE

Yes

If \( T = 60 \)

No

CALL SUBROUTINE 4

CONTINUE

No

CALL SUBROUTINE 5
STORE for display: real time, Logger ID, Black Carbon concentration, Filter Load

If Filter Load > Max Load

No → CONTINUE

Yes → Change Filter, Run in "Zero Air Filter" mode; CONTINUE
Table 1: The comparison of black carbon loading (ng m$^{-3}$) measured by means of an independent optical analysis method with those based on the aethalometer measurements

<table>
<thead>
<tr>
<th>Sample (No. of Days)</th>
<th>Aeth. Data Integ. BC</th>
<th>Optical Analysis</th>
<th>Aeth. Data Integ. BC</th>
<th>Optical Analysis</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 (8)</td>
<td>716.1</td>
<td>784.7</td>
<td>719.7</td>
<td>781.3</td>
</tr>
<tr>
<td>2 (11)</td>
<td>527.6</td>
<td>536.6</td>
<td>520.1</td>
<td>545.7</td>
</tr>
<tr>
<td>3 (8)</td>
<td>1250.3</td>
<td>1253.4</td>
<td>1280.3</td>
<td>1287.8</td>
</tr>
<tr>
<td>4 (9)</td>
<td>555.9</td>
<td>568.5</td>
<td>528.3</td>
<td>563.4</td>
</tr>
<tr>
<td>5 (5)</td>
<td>823.2</td>
<td>853.3</td>
<td>806.6</td>
<td>856.0</td>
</tr>
</tbody>
</table>

Mean ratios of concentrations by methods (Aethalometer / Optical): 0.96

Mean ratios of Concentrations Aethalometer (B/A): 1.01

Standard deviation of Aethalometer (B/A): 0.02

Table 2: The comparison of “Clean air runs’ data obtained for the two aethalometer systems operating in parallel.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Aethalometer A</th>
<th>Aethalometer B</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mean voltage (v)</td>
<td>Standard deviation (v)</td>
</tr>
<tr>
<td>S_D</td>
<td>0.146819</td>
<td>0.000025</td>
</tr>
<tr>
<td>S_L</td>
<td>4.985875</td>
<td>0.000294</td>
</tr>
<tr>
<td>R_D</td>
<td>0.014402</td>
<td>0.000021</td>
</tr>
<tr>
<td>R_L</td>
<td>8.097166</td>
<td>0.000415</td>
</tr>
</tbody>
</table>

Standard deviation of Elemental carbon Concentration (g/m$^3$): 0.0086 0.0080
6.0 Typical data sets and Discussion of results

The typical dataset is represented in Fig 5. In this figure, it is to be noted that two aethalometer were co-located and run in parallel in order to ascertain the reproducibility of their outputs. The following observations could be made:

(a) that both instruments successfully picked air pollution episodes and their responses were perfectly synchronized.

(b) the episodes when air masses came from relatively clean sectors versus polluted sectors could be differentiated based upon the output of the aethalometers. These deductions were corroborated by wind trajectories. For instance northerly air masses originating in the Hudson Bay area see Fig 6 proved to be relatively clean (Day 327, marked "A" on Fig 5) whilst the southerly/westerly air masses (see 5-day back trajectories in Fig 7) picked by the aethalometers on Day 331 (marked "B" on Fig 5) had a very high loading of elemental carbon. Such a high loading cannot be explained by human activities in that remote location on a Sunday is easily understood as resulting from advection from pollutant source regions.

(c) the instrument resolution was very good, as measured by the standard deviations obtained from the clean air runs. It was of the order of $10^{-2}$ μg/m$^3$ (8 ng m$^{-3}$ in Table 2). The instrument’s detection limits are thus below the usual atmospheric perturbations.

(d) the concentrations of black carbon obtained were successfully verified by independent optical analysis. There was very good agreement between these two independent methods (Table 1).

(e) the dataset was in a form that could be uploaded/downloaded to a remote access PC.
120 HOUR TRAJECTORIES
SUN NOV 27 86 12 Z
EGBERT (CARE)

700 MB ▲
500 MB ○
1000 MB □
Conclusions

The aethalometer provides real-time measurement of black carbon concentrations. The temporal resolution of the instrument as well as its precision and accuracy were satisfactory. It provides a tool for assessing anthropogenic contributions even to relatively clean remote locations.
References


NOMENCLATURE

σ - Standard deviation
S – Signal voltage
R – reference voltage
K – Constant
FLO – Flow rate m³/s

Subscripts
L – Lamp on
D – Dark
APPENDIX A

Employing the propagation of errors approach, the error associated with the calculation of black carbon concentration is given by the equation:

\[
\sigma^2_{BC} = 2K^2 \left( \frac{\sigma^2_{SL} + \sigma^2_{SD}}{(S_L - S_D)^2} + \frac{\sigma^2_{RL} + \sigma^2_{RD}}{(R_L - R_D)^2} \right) + \frac{\sigma^2_D}{FLO^2}
\]

APPENDIX B

<table>
<thead>
<tr>
<th>Task</th>
<th>CRZIX command</th>
</tr>
</thead>
<tbody>
<tr>
<td>01 Panel Temperature</td>
<td>P17</td>
</tr>
<tr>
<td>02 Thermocouple Temperature</td>
<td>P14</td>
</tr>
<tr>
<td>03-07 Measure voltages</td>
<td>P2</td>
</tr>
<tr>
<td>08-10 Assignment</td>
<td>P30</td>
</tr>
<tr>
<td>11 Display battery voltage</td>
<td>P10</td>
</tr>
<tr>
<td>12-13 Low Pass filter</td>
<td>P58</td>
</tr>
<tr>
<td>14 Flag setting</td>
<td>P92</td>
</tr>
<tr>
<td>15 Set Resolution to High</td>
<td>P78</td>
</tr>
<tr>
<td>16-17 Set Active Storage Area</td>
<td>P80</td>
</tr>
<tr>
<td>18 Average</td>
<td>P71</td>
</tr>
<tr>
<td>18 Real time</td>
<td>P77</td>
</tr>
<tr>
<td>20 Sample</td>
<td>P70</td>
</tr>
<tr>
<td>21 Maximise</td>
<td>P73</td>
</tr>
<tr>
<td>22 Minimise</td>
<td>P74</td>
</tr>
<tr>
<td>23 Standard Deviation</td>
<td>P82</td>
</tr>
</tbody>
</table>
Figure Captions

Fig. 1  The Schematic Diagram of the Aethalometer (side view).

Fig. 2  The Physical Configuration of Aethalometer

Fig. 3  CIRCUITRY

Fig. 4  Flow chart.

Fig. 5  Aethalometer Field Tests at Egbert November, 1988.

Fig. 6  120 Hour trajectories (Tue NOV 22 88 127) from northerly air masses originating in the Hudson Bay area.

Fig. 7  120 Hour trajectories (SUN NOV 27 88 122) from the southerly Westerly air masses.
OPTIMIZATION FOR NOx REMOVAL IN A NON- THERMAL PLASMA DISCHARGE

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Atlanta, GA 30314

ABSTRACT
Nitrogen oxides (NOx), a group of gaseous pollutants produced primarily by combustion processes, have been shown to contribute to photochemical smog, acid rain and ground-level ozone. As awareness of the detrimental effects of NOx grows, regulations limiting NOx emissions are becoming increasingly more stringent. Non-thermal Plasma Discharge (NTPD) has been identified as a promising technology for NOx removal. As part of a program to optimize a NTPD for NOx removal, an investigation of the effects of discharge gap width, input power, feed gas composition, and residence time on the electrical and chemical processes that occur in a dielectric barrier discharge was undertaken. The experimental methods and results, especially on the effect of gap spacing are presented and discussed.

1.0 INTRODUCTION
The Non-Thermal Plasma Discharge or NTPD provides a means of employing electrical energy to drive selected chemical reactions in contaminated gaseous media (See Figure 1). In one type of NTPD, commonly called a silent discharge or dielectric barrier discharge, the presence of one or two dielectric barriers promotes the creation of plasma channels in non-thermal equilibrium (i.e. microdischarges). In these devices, the electrical energy coupled to the gas is primarily used for the production of energetic electrons, leaving the background gas at ambient temperature. The energy in the plasma is thus directed preferentially to electron-impact dissociation and ionization of the background gas to form free radicals. These free radicals react chemically with the surrounding molecules to produce a more innocuous or compliant effluent.
Figure 1. Schematic of a Typical Double Dielectric Barrier Discharge Device

The NTPD at atmospheric pressure has been applied to the processing of gaseous media for chemical synthesis for many decades.1 Among the most common applications of NTPD is the production of ozone utilizing a single dielectric barrier discharge. In the past several years, the research and use of NTPD technologies has grown significantly. Because of its demonstrated success in creating useful chemical compounds, the NTPD is increasingly being utilized to decompose or breakdown hazardous chemical compounds. For many applications, especially in the removal of very dilute concentrations of air pollutants, the NTPD approach is ideal because it provides energy selectivity and the capability to simultaneously remove several pollutants.2 The focus of this study is on the class of compounds collectively known as nitrogen oxides or NOx.

The release of nitric oxide (NO) into the atmosphere results in its subsequent conversion to nitrogen dioxide (NO2) and eventually leads to a variety of environmental problems. Although NO is colorless, NO2 has a characteristically yellowish-brown color and is largely responsible for the outward appearance of photochemical smog. An ensuing chemical reaction between NO2 and water vapor (H2O) leads to the formation of nitric acid (HNO3) and contributes to acid rain. Furthermore, through an intricate series of reactions involving NO2 and hydrocarbons, high concentrations of ozone (O3) can be formed near the earth's surface. NO and NO2 (photochemical smog), HNO3 (acid rain) and O3 (ground level ozone) are all irritating to the throat and lungs at low concentrations, and potentially lethal at high concentrations.

A primary source of NO emissions is the combustion of hydrocarbon based fuels (such as diesel and JP-8) with air.3 Other potential sources of NO include the disposal of munitions through open burn/open detonation, plasma torch incineration and molten salt oxidation. In order to reduce the hazards associated with NO and NO2 (collectively known as nitrogen oxides or NOx) stringent regulations have been imposed on NOx emissions in many high-risk areas. Because the majority of NOx emissions from Air Force bases within these areas were found to be from diesel powered Aerospace Ground Equipment (AGE), the Air Force began a program called the Green AGE Initiative. The purpose of this initiative was to determine the most effective method to reduce NOx emissions from AGE. An Air Force study conducted under this initiative identified the NTPD as a particularly promising and cost-effective candidate for reducing AGE NOx emissions without compromising the AGE operational constraints.4 The research presented in this
paper was performed in support of an on-going program to optimize the NTPD for this particular application.

Understanding the microdischarge and its relationship with the resulting chemical reactions is the key to developing efficient NTPD technologies. The discharge characteristics are directly related to the electric field maintained between the electrodes of a dielectric barrier device. As increasing voltage is applied to the two electrodes, breakdown is induced once the field within the gap exceeds the corresponding reduced Paschen field. At pressures on the order of 1 atmosphere or higher, the breakdown results in a multitude of filaments or microdischarges having diameters of about 100 μm and lifetimes that are generally less than 100 ns. Both size and lifetime depend on many factors including gap spacing and gas composition. It is important to note that the energy exchanged by collision between accelerated electrons and atoms and molecules occurs entirely within the microdischarges.

Numerous investigations on the influence of gas composition, reduced electric field (E/n) and gas temperature on both emission control and ozone synthesis have been performed. These investigations have utilized various NTPD devices including pulsed corona, surface discharge, and silent (or dielectric barrier) discharge. A great advantage of the silent discharge over many other discharge types is that one can influence the average energy of the generated electrons by changing the product of gas density and gap width. Thus by adjusting the gap width in an atmospheric discharge one can adjust the average electron energy to optimize the yield of the process under study (e.g. NOx removal). The focus of this investigation is on the effect of the discharge gap width on the processes that occur within a double dielectric barrier discharge (DDBD). Our goal is to try to clarify the interplay between physics and chemistry by studying the microdischarge properties and the NO/NOx removal efficiency and their relationship.

The remainder of this paper is organized as follows. In the first section, we describe the experimental set-up and instrumentation. A presentation and discussion of our results follows the experimental section. Finally, in the last section, we submit our concluding remarks and provide recommendations for further study.

2.9 EXPERIMENTS

The NTPD reactor used in our experiments is shown in Figure 2. The reactor, a double dielectric barrier discharge (DDBD) device, consisted of two parallel plate electrodes arranged so that gas entering the device was directed through the gap spacing between the electrodes. The electrodes were constructed by sealing a thin aluminum mesh between two 1/32" thick, tempered Pyrex glass plates with a silicon sealant. Electrical connections to the aluminum were made by stripping and flattening the end of a piece of 16 gauge stranded copper wire and inserting the flattened wire between the plates prior to sealing. The active area of two adjacent electrodes was approximately 50 square centimeters.
The DDBD reactor housing (shown in Figure 2) was made of PVC with ports for the inlet and outlet gas flows and the high and low voltage terminals. Plexiglass and rubber shims were used inside the reactor housing to ensure that no gas flow occurred outside of the reaction zone. The top and bottom of the reactor housing were sealed with an o-ring and a Plexiglass cover. Teflon spacers of well-defined thickness separated the electrodes in order to fix the size of the gap spacing. The gap thickness was varied between 0.8 and 4.0 mm in the experiments.

A schematic of the overall experimental setup is given in Figure 3. The power supply was a model 501SL-12/401SD-002 AC Power System manufactured by Elgar Corporation and capable of delivering 0-260 Volts at frequencies of 45 to 5000Hz. A 3-kVA transformer with a nominal step-up of 70:1 at a frequency of 400Hz was used. A Hewlett Packard 54600 oscilloscope with four channels was employed in the experiments to measure the voltage, charge, and current versus time. Due to the high voltage, two Tektronix P651 high voltage attenuation probes (x1000), were connected between the oscilloscope and the voltage terminals. The charge was measured using a 1 uF sense capacitor and the current was detected via a Pearson Model 101 current transformer. By connecting the oscilloscope to a PC with a GPIB PCI II card, data was transmitted to the PC and subsequently used to calculate the power consumption and other system parameters.

An 8-channel digital thermometer measured the temperatures of the inlet flow, outlet flow, and surroundings, while a U-tube manometer was employed to measure the pressure drop across the DDBD. The gas matrix was fed quantitatively, using MKS 1179 Mass-Flow Controllers, from gas cylinders of O₂, N₂, and NO (with N₂ balance). A vapor generator was used to provide the desired level of water vapor in the inlet gas stream. The post-reaction outlet flow
gases were analyzed for NO and NO{sub}x using a Horiba CLA-510s chemiluminescence gas analyzer with 1% accuracy. A Perkin-Elmer Spectrum 2000 FTIR with a 20 m variable path gas cell and a Shimadzu GC 17-A/QP2000 GC-MS were also utilized to quantitatively monitor products after DDBD processing.

\[ \text{Figure 3. Schematic of Experimental Setup} \]

A KODAK EKTAPRO High Speed Intensified Imager System and Nikon Micro lens were used to study the microdischarges. Specifications for the camera system include a frame rate of 30-6000 fps, a spectral sensitivity of at least 50% peak from 440 nm to 700 nm, and a variable gate time from 10-5000 μsec. Output from the imaging system was recorded on videotape via a 1/2” VHS VCR. The system was used to view the microdischarges from points both perpendicular and parallel to the breakdown channel.

3.0 RESULTS

Various measurements were made using the system described in the previous section. The different measurements can be grouped into three categories: (1) breakdown voltage, (2) NO{sub}x removal, and (3) microdischarge observations. The breakdown voltage provided essential information regarding the electric field strength under which the discharges occur. The NO{sub}x removal measurement, along with measurements of the input power and gas flow rate, provided system level information relating to the performance of each gap width. The optical measurements obtained by the high-speed imager provided valuable qualitative information about the microdischarges. Each of the measurements is discussed in detail below.

4.0 BREAKDOWN VOLTAGE

One of the most important physical aspects effecting the microdischarge is the breakdown voltage, \( V_b \). As a rising voltage is applied to the gap, electron avalanches begin propagating from the cathode toward the anode. Due to the high \( nd \) (product of gas density \( n \) and gap spacing \( d \))
value, a considerable space charge is generated during the first avalanche's first transit through the gap. As voltage grows further, secondary processes such as the creation of electrons by particles resulting from the primary process of electron impact ionization come into play. Secondary processes affect amplification more strongly if they produce electron emission from the cathode. With secondary emission taken into account, the steady discharge current, \( I \), is given by:

\[
I = \frac{I_a e^{\alpha d}}{1 - \gamma (e^{\alpha d} - 1)}
\]  

(1)

where \( \alpha \) designates the number of ionizing collisions, \( \gamma \) the effective secondary emission coefficient for the cathode, and \( d \) the gap spacing. For flat electrodes with a uniform field distribution, the coefficient of ionization increases with decreasing gap width. This is a criterion for the occurrence of a self-sustaining discharge, which has the following form:

\[
I \to \infty, \quad \alpha d = \ln \left( \frac{1}{\gamma} + 1 \right)
\]  

(2)

In Equation (2) \( \alpha = Ap \cdot \exp(-Bp/E) \) where \( p \) is the pressure, \( E \) is the electric field given by \( E = V_a/d \) and \( A \) and \( B \) are constants which depend on the gas and the cathode material, respectively. Thus \( \alpha \) depends on the gas, the material of the cathode, the pressure, and the discharge gap spacing. To arrive at explicit expressions, we substitute \( \alpha \) and \( E \) into Equation (2), to obtain

\[
V_a = \frac{Bpd}{\ln pd + \ln \left( \frac{A}{\ln \left( \frac{1}{\gamma} + 1 \right)} \right)}
\]  

(3)

In our case, the applied voltage, \( V_a \), at breakdown is, \( V_a = V_b + 2V_e \), where \( V_b \) is the voltage on the dielectrics. The dielectric voltage is \( V_d = V_b \left( C_{ion} / C_{die} \right) \) so in terms of the dielectric constant of the dielectric material Equation (3) becomes

\[
V_d = \frac{Bpd \left( 1 + \frac{2t}{Kd} \right)}{\ln pd + \ln \left( \frac{A}{\ln \left( \frac{1}{\gamma} + 1 \right)} \right)}
\]  

(4)

where, \( t \) is the thickness of the dielectric and \( K \) is its dielectric constant. Taking \( 1/\gamma \) and \( p \) to be constant, we can write
\[ V_x = \frac{C_1 d + C_2}{\ln d + C_3} \]  \hspace{1cm} (5)

where

\[ C_1 = Bp \]

\[ C_2 = \frac{218p}{K} \]

\[ C_3 = \ln \left[ \frac{Ap}{\ln \left( \frac{1}{\gamma} + 1 \right)} \right] \]

The experimental breakdown (or Paschen) curves along with a numerical fit of Equation (5) to the experimental data are plotted in Figure 4. The constants for the fit were found to be \( C_1 = 12339 \) volts/mm, \( C_2 = 9254.7 \) volts, and \( C_3 = 4.1 \).

\[ \text{Figure 4. Relationship Between Breakdown Voltage And Gap Width,} \]
\[ \text{Pressure: 1 atm, Temperature: 22.5°C, Residence Time: 0.5 s,} \]
\[ \text{Gas Composition: 1000 ppm NO, 2000 ppm H}_2\text{O, 10% O}_2, \text{N}_2 \text{ balance} \]

As shown in Figure 4, the experimental values for the breakdown voltage are fit well by the functional form predicted by the theoretical considerations (i.e. Equation 5). The breakdown voltage can be used to establish the electric field for the microdischarges through the relation 

\[ \frac{V}{d} = \frac{E_b}{n}. \]

NO\(_x\) removal

In gas streams containing appreciable amounts of both oxygen and NO (e.g. diesel exhaust), the primary effect of NTPD treatment is the oxidation of NO to NO\(_x\). NO\(_x\) removal is then attained through the removal of NO\(_x\) by either catalytic reduction or wet scrubbing. The effectiveness of the NTPD in removing NO\(_x\) is therefore fundamentally tied to its ability to remove (or oxidize) NO. In Figure 5 the quantity of NO removed from the gas stream is plotted against the energy deposition for gap widths ranging from 0.8 to 4.0 mm. For these tests, the gas stream makeup was fixed, consisting of 1000 ppm NO, 2000 ppm H\(_2\)O, and 10% O\(_2\) with N\(_2\) as the balance gas. The energy deposition was determined from the input power (sense capacitor) and the gas flow rate (mass flow controllers). The NO concentration was measured before applying
power to establish the initial concentration and then measured at subsequent power levels to determine the amount of NO removed. The residence time of the gas within the NTPD reactor was fixed and all tests were performed at atmospheric pressure and room temperature. To maintain a fixed residence time (≈ 0.5 s) while varying the gap width, the gas flow rate to the reactor ranged from 0.667 L/min to 3.33 L/min.

![Figure 5](image)

**Figure 5**  
NO removal versus Energy Deposition  
Pressure: 1 atm.  
Temperature: 22.5°C,  
Gas: 1000ppm NO, 2000ppm H₂O, 10% O₂, N₂ balance.

In this investigation, the DDBD test device was relatively effective at removing (i.e. oxidizing) NO from the mock combustion gas stream. The percent of NO removed from the gas stream in our tests ranged from 20% to 40% with input powers from 0 to 6 Watts. As seen in Figure 5, the performance of all gap widths fell into a narrow range at low energy deposition but widened considerably for higher energy depositions. By comparing the amount of NO removed by each gap width at similar energy depositions, the optimum gap width could be determined. The result of this analysis is shown in Figure 6 for a typical energy deposition of 150 mJ/cc. Notice that the best NO removal was observed at a gap width of approximately 2 mm. The error bars shown in Figure 6 represent an estimated 5% error in measuring the NO concentration and an estimated 1% error in setting the gap width. The dashed curve in Figure 6 has no physical basis but is provided to illustrate the general trend of the data.
Figure 6. NO Removal versus Gap Width, Pressure: 1 atm
Temperature: 22.5°C, Gas: 1000ppm NO, 2000ppm H2O, 10% O2, NO balance.

The standard of performance for pollution control devices is the energy required to remove a given quantity of pollutant. In the case of electrical devices removing dilute concentrations of pollutants, the performance is best described in terms of the number of eV required to remove each pollutant molecule. Given in Table 1 are the efficiencies for each gap width we tested at energy depositions of 50, 100 and 150 mJ/cc. The efficiencies are given in terms of eV per NO molecule removed (or oxidized). Note that the 2 mm gap width outperformed all other gap widths over the range of energy depositions considered. Also note that the NO removal efficiency decreases (i.e. the eV per molecule increases) with increasing energy deposition.

Table 1: NO removal efficiency at various gap widths and energy depositions

<table>
<thead>
<tr>
<th>Gap Width, d (mm)</th>
<th>Energy Deposition 50 mJ/cc</th>
<th>Energy Deposition 100 mJ/cc</th>
<th>Energy Deposition 150 mJ/cc</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.3</td>
<td>82</td>
<td>100</td>
<td>133</td>
</tr>
<tr>
<td>1.5</td>
<td>92</td>
<td>101</td>
<td>125</td>
</tr>
<tr>
<td>1.6</td>
<td>76</td>
<td>94</td>
<td>121</td>
</tr>
<tr>
<td>2.0</td>
<td>74</td>
<td>92</td>
<td>114</td>
</tr>
<tr>
<td>2.4</td>
<td>82</td>
<td>97</td>
<td>124</td>
</tr>
<tr>
<td>2.5</td>
<td>94</td>
<td>109</td>
<td>134</td>
</tr>
<tr>
<td>3.0</td>
<td>103</td>
<td>114</td>
<td>136</td>
</tr>
<tr>
<td>3.2</td>
<td>86</td>
<td>112</td>
<td>142</td>
</tr>
<tr>
<td>3.5</td>
<td>92</td>
<td>109</td>
<td>130</td>
</tr>
<tr>
<td>4.0</td>
<td>101</td>
<td>125</td>
<td>142</td>
</tr>
</tbody>
</table>

5.0 MICRODISCHARGE OBSERVATIONS
Photographs, which were taken with the intensified high-speed imager in framing mode, revealed details of the microdischarge behavior. The spectral range of the imager was from 400 to
800 nm and we assumed that the microdischarge images in this range represent the primary electron stream forming the discharge channel. It is important to note that the duration of the discharge image reflects only the integration of the excimer's life within the channel and not the duration of actual charge transfer through the channel. During a single half power cycle both the number and the physical dimensions of the microdischarges could be obtained directly by the imager. In order to extract further information from the optical observations the characteristics of the microdischarges were related to the transferred charge. For this analysis the DDBD’s electrode configuration was presumed to be symmetric and we further assumed that all of the available surface charge was transferred through microdischarges in which chemical reactions were initialized. The specific reactions taking place within the microdischarges are determined by electron-molecular/atom collisions.

The planar DDBD arrangement used in the experiments and the geometry assumed for the microdischarges are shown in Figure 7. The microdischarge consists of a small channel both between and perpendicular to the electrodes as well as a creep discharge or footprint on the dielectric surface. For simplicity, a cylindrically shaped channel with radius r and a disc shaped footprint with radius R_s are defined as shown in Figure 7. Power is input into the DDBD by applying a sinusoidal voltage waveform of sufficient amplitude to initiate discharge. During the discharge process, a dielectric double layer is built up at the dielectric surface. This layer reduces the field strength within the gap leading to extinction of the discharge within a few nanoseconds. Multiple discharges occur during each half cycle of the applied voltage waveform. At a given gap width, increasing the voltage increases the number of discharges and therefore the input power.

![Figure 7. Arrangement of the DDBD and Sketch of a Simplified Microdischarge](image)

A series of microdischarge images at different gap widths are presented in Figure 8. When obtaining these images, the residence time of the gas in the DDBD device was fixed. The fixed residence time was accomplished by changing the inlet flow rate when changing the gap spacing. The input power, driving frequency, and flow temperature were also fixed in each case, as was the gas mixture.
Figure 8. High-Speed Images of Microdischarges at Different Gap Widths.

Gas composition: 1000 ppm NO, 2000 ppm H₂O, 10% O₂, N₂ balance,
Room Temp, 1 atm, Power=5 Watts, Frequency=400 Hz, Residence
time=0.46 s

The specific conditions under which the images in Figure 8 were obtained are given in the figure caption. Notice that with increasing gap spacing the radius, r, of the discharge increased significantly, while the number of discharges per half cycle dramatically decreased. The radius was found to vary from approximately 90 μm at the 1 mm gap width to 340 μm at the 4 mm gap width. The frame rate for these images was 1000 fps and the gate time was varied from 20 to 200 μs to obtain the clearest image.

In addition to affecting the radius of the microdischarge channel, the gap width significantly affected the footprint of the discharge. The radius of the footprint, Rφ, increased with gap width even more markedly than the channel radius. The footprint radius was approximately 100 μm at 1 mm gap width while it grew to 1700 μm at the 4 mm gap width. The footprint extended only slightly beyond the channel at the smaller gap width but was many times the channel radius at larger widths. Despite being significantly affected by the gap width, both the channel radius and the footprint radius were largely unaffected by variations in the input power.

The other major effect observed when varying the gap width was the number of discharges. As the gap width was decreased the number of discharges increased significantly. By taking high-speed photographs of the discharges through the glass and aluminum mesh, it was possible to estimate the number of discharges per half cycle for each gap width. At an input power of 5 Watts, we estimate that there were approximately 7000 discharges per half cycle for the 1 mm gap width while for a gap width of 4 mm the number of discharges was only 400 per half cycle. Since the input power was fixed, the decrease in the number of discharges with increasing gap width implies that the mean charge per discharge increases with increasing gap width. This is supported by our observation that the photo intensity of individual microdischarges increased with increasing gap width at fixed input power.
Table 2 summarizes the information that we were able to derive from the optical measurements. It should again be noted that the measurements are based only on the wavelength range visible to the camera, i.e. 400 to 800 nm.

Table 2. Summary of microdischarge properties derived from optical measurements.

<table>
<thead>
<tr>
<th>Gap Width, d (mm)</th>
<th>Discharge Radius, r (μm)</th>
<th>Footprint Radius, R₀ (μm)</th>
<th>Number of Discharges per Half Cycle, n</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>90</td>
<td>100</td>
<td>7000</td>
</tr>
<tr>
<td>2</td>
<td>170</td>
<td>500</td>
<td>2000</td>
</tr>
<tr>
<td>3</td>
<td>230</td>
<td>1300</td>
<td>700</td>
</tr>
<tr>
<td>4</td>
<td>340</td>
<td>1700</td>
<td>400</td>
</tr>
</tbody>
</table>

In obtaining the data presented in Table 2, the experimental conditions were kept as constant as possible by utilizing identical gas mixtures, residence times, driving frequencies, temperatures, pressures and input powers. All of the observations were made under approximately atmospheric conditions (i.e. T = 22 °C, P = 1 atm). Since the microdischarges initialize the chemical reactions that drive the NO removal process, the properties of the microdischarges are key to the performance of the NTPD. The data presented in Table 2 were utilized to determine the variation of significant discharge characteristics (i.e. the microdischarge and footprint radius) with gap width.

Figures 9 and 10 show the experimental results obtained from the optical measurements of the microdischarges at different gap widths. The microdischarge radius, which was obtained directly from the discharge images, is plotted against the gap width in Figure 9. An approximately linear relation between the radius of the microdischarge, r, and the gap width, d, was obtained. The equation for a linear fit of the data is given in Figure 9. Note that since the y-intercept of the fit is relatively small, we can adopt a simple estimate for the radius of 80 μm per mm of gap width.
Due to the high local eigen-field, the high-energy tail electrons of the avalanche along the electrode surface can be accelerated to high velocity. These high-energy electrons collide with molecules close to the surface and form a footprint to the microdischarges as they propagate toward the breakdown channel. The radius of the footprint was measured at each gap width and is plotted in Figure 10. Again, a linear relationship was observed as evidenced by the figure.

The equation for the linear fit of the data shows that the slope (560 \( \mu \text{m per mm} \)) is quite large and that the y-intercept (-500 \( \mu \text{m} \)) is far below zero. The large slope indicates the gap width affects the footprint radius more strongly than it affects the discharge radius and the negative slope may further indicate that the actual radius of the footprint is larger than the radius viewed by the camera.
6.0 DISCUSSION

Our results indicate that at constant power input, the charge transferred through individual microdischarges increases with increasing gap width while the number of microdischarges decreases. Because the increase in charge transferred is accompanied by an increase in discharge size, the affect of gap width on the volume charge density within the microdischarge has not been directly established. The microdischarge charge density is directly related to reaction rates within the discharge and may be a good indicator of overall performance. If we assume that all of the surface charge contained in the area of the footprint is transferred into the microdischarge channel, the volume charge density within the microdischarge channel can be roughly estimated. This assumption can be stated simply as

\[ \sigma A = \rho V, \]

(6)

where \( \sigma \) is the surface charge density, \( A \) is the area of the footprint, \( \rho \) is the volume charge density within the discharge channel and \( V \) is the volume of the discharge channel. Assuming a cylindrical footprint and circular footprint, Equation (6) reduces to

\[ R_o = \left( \frac{\rho d}{\sigma} \right) r. \]

(7)

Equation (7) suggests a linear relationship between the footprint radius and the discharge radius. Figure 11 shows a plot of \( R_o \) versus \( r \) for our experimental values. Indeed a linear relationship was observed when plotting these two quantities against each other.

![Figure 11. Plot of the Footprint Radius, \( R_o \) versus the Microdischarge Radius, \( r \).](image)

The equation for the linear fit to the data is given in Figure 11 and the slope determined from this fit can be equated with the bracketed quantity in Equation (7) to estimate the volume charge density of the microdischarges. To solve for the volume charge density we must first specify the surface charge density. The surface charge density at each gap width is directly related to measurable quantities and can be found from the equation,
\[ \sigma = \frac{C_{\text{die}} V_{\text{die}}}{A_{\text{die}}}, \]  

where \( C_{\text{die}} \) is the capacitance of the dielectric, \( V_{\text{die}} \) is the voltage on the dielectric and \( A_{\text{die}} \) is the area of the dielectric. The equation for the volume charge density is thus determined from the equation

\[ \rho = \frac{k^2 C_{\text{die}} V_{\text{die}}}{dA_{\text{die}}}, \]

where \( k = 6.89 \) is the slope of the \( R_s \) versus \( r \) curve. In Equation (9) only \( V_{\text{die}} \) is dependent on the gap width and has to be determined experimentally. Values for \( V_{\text{die}} \) were taken from the experimental values of the applied voltage and the breakdown voltage (discussed in an earlier section). The results of this analysis are given in Table 3. In addition to the volume charge density, the corresponding electron density is also given in Table 3. The estimated electron density values are consistent with values suggested in the literature.\(^5\)

<table>
<thead>
<tr>
<th>Gap Width, ( d ) (nm)</th>
<th>Dielectric Voltage, ( V_{\text{die}} ) (V)</th>
<th>Volume Charge Density, ( \rho ) (C/m(^3))</th>
<th>Electron Density, ( n_e ) (( \times 10^{15} ) cm(^{-3}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3121</td>
<td>3.47</td>
<td>2.17</td>
</tr>
<tr>
<td>2</td>
<td>2047</td>
<td>1.14</td>
<td>0.71</td>
</tr>
<tr>
<td>3</td>
<td>1597</td>
<td>0.59</td>
<td>0.37</td>
</tr>
<tr>
<td>4</td>
<td>1362</td>
<td>0.38</td>
<td>0.24</td>
</tr>
</tbody>
</table>

As seen in Table 3, our analysis suggests that the microdischarge charge densities increase with decreasing gap spacing. This would indicate that electron-impact dissociation and ionization of the background gas to form free radicals is favored for smaller gap widths. However, through the coupling of gas analysis with detailed information on system electrical parameters, the peak processing efficiency (for NO removal) of our NTPD system was found to be near the center of the range of gap widths tested. The observed optimum is attributable to the large number of factors (including the chemical composition of the gas stream, the charge density of the microdischarges, the electron energy distribution in the microdischarges and the distribution of microdischarges within the reactor) that determine the overall NO removal efficiency. Since many of the parameters affecting NO removal in an NTPD are dependent on the gap width, it is not unexpected that an optimum gap width exists for this process. Given the large number of factors affecting performance, it is probable that for each particular stream makeup a different optimum gap width exists.

Although we have not yet established the physical basis for the optimum, we have identified some possible explanations. At the larger gap widths where there are considerably fewer discharges the volume of gas subjected to reactions with short-lived radicals within the discharge may be limited resulting in poor performance. In addition, as the gap width increases
the average electron energy and charge density within the microdischarges decreases, resulting in fewer ionizing collisions. In the case of smaller gap widths, the average electron energy, charge density and volume of gas subjected to radical reactions are increased, however, these factors may lead to the intensification of processes that produce NO or convert NO\textsubscript{2} back into NO. Both direct dissociation of NO\textsubscript{2} by high-energy electrons and dissociation of NO\textsubscript{2} via UV absorption are candidate processes that may lead to reduced performance at smaller gap widths. Since the physical basis for the existence of an optimum gap width is not yet well understood, determining the nature of the optimum will be the focus of our future efforts.

7.0 CONCLUSION

Non-thermal plasma discharges are increasingly being utilized for the processing of hazardous gas streams. As the technology matures, research must focus more and more on the system level effect of various operating parameters. Our study indicates that gap width can be considered one of the major factors affecting the physical properties and performance of dielectric barrier discharges. In order to evaluate the effect of gap width on NO removal in combustion gas streams, both the physical properties of the microdischarges and the NO removal efficiency were investigated at gap widths ranging from 0.8 to 4.0 mm. Photographic studies showed that the radius of both the microdischarge footprint and cylindrical channel increased linearly with gap width while the number of discharges decreased with increasing gap width. Additionally, by relating the surface charge within the footprint to the charge contained in the discharge channel an estimate of the microdischarge charge density was obtained. System level measurements of the NO removal efficiency at various gap widths revealed that for the selected gas stream the NO removal peaked at a gap width of approximately 2 mm. Physical considerations suggest that for larger gap widths the reduced electron energy, charge density and spatial coverage of the microdischarges limits effectiveness while at smaller gap widths the reverse trends lead to intensification of processes that adversely affect NO removal. Although the observed optimum gap width is potentially only applicable to our specific test conditions, the existence of an optimum indicates that each application of NTPD to toxic gas removal may benefit from consideration of the gap width. An understanding of the development and properties of the microdischarges in a NTPD are key to interpreting the relationship between the physical and chemical performance of these devices. Further efforts are needed to establish the physical basis for the observed optimum gap width and clarify the role the gap width plays in determining both the microdischarge characteristics and subsequent chemical processes.

8.0 ACKNOWLEDGMENTS

The authors gratefully acknowledge the support of the Munitions Division of the Air Force Research Laboratory Munitions Directorate (AFRL/MNM) at Eglin AFB, Florida under Contract #F08630-96-K-0015, and the Department of Defense under Grant No. N00014-97-1-0511.
9.0 REFERENCES

OPTICAL TECHNIQUES FOR DIAGNOSTICS OF COMBUSTION AND ATMOSPHERIC ANALYSIS

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ABSTRACT

Optical diagnostics techniques are the most powerful tools for the understanding of combustion processes and the detection of combustion products. Their main advantages are related to the minimal perturbation induced to the system, and to the non contact probing, which allows measurement in extreme temperature, pressure, and chemical environment, as found in flames and all other combustion processes. Many optical interaction processes between optical radiation and gases can be used for this purposes, including emission, absorption, fluorescence, elastic and inelastic scattering. This presentation will review these processes, the experimental techniques, and the relative equipment, focusing on the simplest measurements which can be easily performed in the laboratories in developing countries. Some of the measurement will be also proposed as training experiments, suitable to be performed with the equipment already existing in the Laser and Fibre Optics Centre of the University of Cape Coast. Indications will also be given on how to design, build and calibrate simple systems, like an optical pyrometer and an infrared radiometer, with minimal investment, using readily available parts and components.

1.0 OPTICAL MEASUREMENTS

1.1 Emission measurements

All the above mentioned interaction processes with the optical radiation are of use for diagnostics, starting from the most basic linear processes, emission, absorption and scattering. Actually emission is the simplest optical technique that can be used for combustion monitoring. For example ignition of fire is almost always detected by the emission of light.

The emission of light by any object is basically dominated by temperature. Often, especially in the infrared region of the spectra many objects can be considered as blackbodies, then the emission spectrum $W_\lambda$ is dependent only on the absolute temperature $T$, as given by the Planck's law:

$$W_\lambda = \frac{2hc^2}{\lambda^5} \frac{1}{\exp\left(\frac{hc}{\lambda kT}\right) - 1}$$

The measurement of the emission spectrum is then a good...
measurement of the temperature of the emitter. The blackbody temperature can be also retrieved without performing the spectra. Integration of the Planck's law gives the total emission of a blackbody, known as the Stefan–Boltzmann law:

$$W_T = \sigma T^4$$  \hspace{1cm} (2)

If the emission is not that of a blackbody, sometimes the spectral shape still remains the same. In that cases the emitter is called a greybody, and the emission is proportional to that of a true blackbody by a coefficient $\varepsilon$ ($0 < \varepsilon < 1$), which is called emission coefficient. This is close to unit, especially in the infrared for most dielectrics, while conductors have much lower emission ($\varepsilon < 0.1$).

Once the material of the emitter is known its temperature can be still retrieved taking into account its emission coefficient, which is reported in tables for the most common materials, in the above relations. The Stefan–Boltzmann law becomes, for example:

$$W_T = \varepsilon \sigma T^4$$  \hspace{1cm} (3)

To achieve a reliable temperature measurement the spectra must be performed close to the peak of the emission, which is given by the Wien's law.

$$\lambda_{\text{max}} = \frac{2896}{T} [\mu \text{m}]$$  \hspace{1cm} (4)

This is another method to retrieve the temperature from the blackbody spectrum, but only gives indication of the temperature range where the emission becomes visible to the human eye ($380 < \lambda < 780$ nm).

In this range the naked eye is also the base of a simple instrument, the optical pyrometer, which allows contactless temperature measurement by using the emission colour of an hot (> 500 C) object which emits light. It is made from a small magnifying optical device (like a monocular) in which a small incandescent light bulb is placed. The filament image is seen by the user with the hot object to be gauged as background. The electrical current flowing through the filament in the bulb is controlled by a potentiometer until the top (hottest part) of the bulb filament almost disappears. The temperature of the filaments is then the same of the background and the current is read on a calibrated ammeter. This device can be easily built modifying half of a used small binocular, just inserting the bulb in a suitable position.

The optical pyrometer, and all other instruments measuring blackbody emission, are quite useful devices when measuring the temperature of hot solid bodies. In combustion control applications they are then mainly useful for the temperature measurement of furnaces, melts, or
other solid objects heated by the flame. When directly used for the measurement of flames the fact that the emission spectrum of a gases is usually quite different from that of a blackbody must be taken into account. Light emitted from a hot gas comes mainly from electronic transitions. Three processes lead to light emission when an electron loses energy: a free electron lose energy, but remains free (free-free transition), or it remains bound to an ion (free-bound) transition. The other process is a transition from a upper to a lower bound state. While the first two processes are not quantized, thus leading to a continuum spectrum, the latter process is discrete and the spectrum is made of separate lines, as shown in Fig. 1.

![Diagram showing transitions between free-free, free-bound, and bound-bound](image)

**Fig. 1**

The emission spectrum of a hot gas is then a combination of lines and continuum and the blackbody formulas cannot be applied directly. The measurement of the total emission usually results in the evaluation of soot temperature, in the carbon particles heated by the flame.

The gas emission can be still used for flame diagnostics, but a spectrometer delivering the necessary resolution to distinguish between lines and continuum is necessary. The relative line intensities can still deliver the information on temperature, since the population of the levels is dependent on temperature, by the Boltzmann distribution:

\[
\begin{align*}
N_2 & = N_1 \exp \left( - \frac{(E_2 - E_1)}{kT} \right) \\
\text{But even more information can be extracted by the analysis of the line profiles. This can be done in emission, but it is often difficult to extract the true line profile from the continuous background emission produced by soot and by the gas itself.}
\end{align*}
\]
1.2 Absorption measurements

The lineshape can be measured much more easily by absorption spectroscopy. Absorption gives also more quantitative information about concentration of the gas species found in the absorption path, making use of the Lambert-Beer law:

\[ I_l(\lambda) = I_0(\lambda) \cdot e^{-\alpha_m(\lambda)lc} \]

Where \( I \) is the absorption, \( I_0(\lambda) \) is the incident intensity, \( c \) is the concentration of the absorber, and \( \alpha(\lambda) \) is the molar extinction coefficient of the investigated line.

The molar extinction coefficient contains the lineshape information for a given species and transition. It is usually divided into two parts as follows:

\[ \alpha_m(\nu) = S(T) \cdot g(\nu - \nu_0, P_{tot}, P_{par}, T) \]

\( S(T) \) is the so-called oscillator strength, and its value for many species and transitions is found in databases. The most important one is HITRAN (High resolution Transmission database) containing more than one million lines. The database is currently distributed on a single CD-ROM free of charge to researchers for their institutional purposes. It can be requested by completing the HITRAN Request Form in Internet from the website www.hitran.com. HITRAN also contains a compilation of spectroscopic parameters which a variety of computer simulation codes use to predict the transmission and emission of light in the atmosphere, files containing aerosol indices of refraction, UV line-by-line and cross-section parameters, supplemental files of gases such as ionic species and high-vibrational calculations, and more extensive IR cross-sections. In addition, there is the software for handling of the data in both Windows and UNIX platforms.

The dimensionless function \( g(\nu) \) is the normalized spectral lineshape function, that is:

\[ \int g(\nu) d\nu = 1 \]

For a single, isolated, line two different lineshape functions are normally possible, depending on the transition and the temperature and pressure conditions.

At low pressure the line is broadened mainly by the doppler mechanism, and lineshape results gaussian:

\[ g(\nu) = \frac{2}{\Delta \nu \sqrt{\ln(2)}} \exp \left[ - \left( \frac{\nu - \nu_0}{\Delta \nu/2} \right)^2 \ln 2 \right] \]

where

\[ \Delta \nu = 2\nu_0 \left( \frac{2kT}{Mc^2} \right)^{1/2} \]
At higher pressures the line is broadened mainly by the collision mechanism, and lineshape results lorentzian:

\[
g(v) = \frac{1}{2\pi} \left( \frac{\Delta v}{(v - v_0)^2 + (\Delta v/2)^2} \right)
\]

where

\[
\Delta v = \frac{1}{\pi \tau}
\]

With \( \tau \) = the level lifetime, usually determined by the collisions.

In intermediate conditions of pressure and temperature both broadening mechanisms are present, and the resulting lineshape is a linear combination of the lorentzian and gaussian profile, known as the Voigt function.

2.0 Tunable Diode Laser Spectroscopy

The measurement of the absorption spectra can be done with a broadband source and a spectrometer, or a interferometer. However, with a flame this is made difficult by the broadband emission of the flame itself.

---

**Fig. 2:** Broad Band Spectroscopy Set up

**Fig. 3:** Laser Spectroscopy Using a Tunable Laser
Using a laser as light source gives the advantage that its high brilliance easily overtake the flame emission. Using a tunable laser, as shown in the picture, the spectrometer becomes also unnecessary. Tunable lasers are usually complex and expensive, but recently the technology of semiconductor lasers succeeded in producing low cost, uncooled, diodes with sufficient resolution to resolve single absorption lines of gases. Tunable Diode Laser Spectroscopy (TDLS) is then becoming one of the most common technique for gas spectroscopy. The rapid scan possibility of such devices, up to the MHz range, also improve the rejection of noise, using detection schemes as the Wavelength Modulation Spectroscopy (WMS).

The wide choice of semiconductor materials make possible the continuous coverage of most visible and near-to-mid infrared region of the spectra, where most of the absorption lines of the molecular species lies. The following table reports the possible technologies to achieve the wanted wavelength. Cooled operation with cryogenic liquids (mainly liquid nitrogen) is necessary now only for semiconductors based on lead salt, at wavelengths longer than about 4 μm. At shorter wavelengths, a temperature stabilisation with thermoelectric coolers is usually sufficient.

In addition to the flame diagnostics the TDLS technique is also being applied in atmospheric analysis. Its high sensitivity allows detection of trace gases and pollutant in the even in the ppb range.

Table 1: Semiconductor Materials with its Emission Spectral Ranges
3.0 Differential Optical Absorption Spectroscopy

For environmental applications the advantage of the TDLS in rejection of the unwanted light is much less needed, then spectroscopy with broadband sources can be used. The simplest optical remote sensing techniques is the Differential Optical Absorption Spectroscopy (DOAS). This technique requires relatively simple and low cost experimental systems, so it is particularly suitable for developing countries.

The equipment as shown in Fig.4 consists of a Xenon short arc lamp which is collimated by a small telescope. A receiver is located at a distance from 0.5 to 5 km, measuring the absorption of the gas in between. A grating spectrometer coupled to a second telescope measures the spectra. Rapid scanning of the whole spectral region of interest is required to prevent the spectrum to be blurred by the atmospheric turbulence, the so called scintillation. More recently this problem is overcome by the use of a CCD detector, which measures all the spectrum simultaneously.

DOAS can be also performed using Sun as light source. In this case horizontal measurement, like pollution over an urban area can be performed only at sunrise or fall.
LASER TECHNIQUES IN COMBUSTION AND FLAMES
PRINCIPLES OF LASER DIAGNOSTICS FOR COMBUSTION

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ABSTRACT

Linear and non-linear optical diagnostic methods are outlined to explain the underlying physical principles. Laser Induced Fluorescence, LIF; Coherent Anti-Stokes Raman Scattering, CARS; Degenerate Four Wave Mixing, DFWM and related laser induced grating methods together with Polarisation Spectroscopy, PS, are reviewed. The measurement of the important combustion parameters, especially temperature and species concentration, using these techniques is outlined. Applications of these techniques to measurements in flames and engines are described to illustrate their operation and relative merits for particular situations.

1.0 INTRODUCTION

Laser techniques offer the important advantages of remote and non-invasive sensing for diagnostics of combustion [1]. The disturbance to hydrodynamic flows inherent in the use of physical probes such as thermocouples or sample tubes is avoided. Furthermore the surface catalytic effects on the chemistry of flames is also avoided and transient species such as radicals may be detected in situ. Laser and optical techniques fall into two broad categories: linear and non-linear. Linear techniques rely on spontaneous emission of radiation from laser excited molecules. Non-linear methods use coherent interactions to produce laser-like signal beams. These methods can be applied to measurements using species present either as major or minor constituents. Major species in air-fed combustion are present in concentrations of more than 1% such as nitrogen, oxygen, carbon dioxide and water. Minor species may be present in only very low concentrations at the parts per million level or lower eg. OH, C2, CH, NO, HCO, CH3. Linear methods such as spontaneous Raman or Rayleigh scattering can only be used with major species owing to their low scattering efficiency. However Laser Induced Fluorescence, LIF, is a resonant process and capable of detecting minor species. Under ideal conditions it is even capable of detecting single atoms! However the LIF signal is weak and radiated into 4π solid angle making detection inefficient and difficult to discriminate against other scattered laser light or flame luminosity. The non-linear process of Coherent Anti-Stokes Raman Scattering, CARS, produces a laser-like beam that allows excellent discrimination against flame emission or scattering and can be collected with almost 100% efficiency. The main drawback of CARS is that it is suitable only for major species and does require two separate laser systems. The coherent advantages of CARS and the resonant sensitivity of LIF are provided by Degenerate Four Wave Mixing, DFWM, making it a useful tool for measurements in minor species in luminous environments. DFWM is one of a class of optical methods which operate by inducing a grating-like structure in the medium. Some other Laser Induced Grating Spectroscopy, LiGS, methods offer particular
advantages in some important respects. Polarization Spectroscopy, PS, provides similar advantages to DFWM with some technical disadvantages for application in practical situations.

In these two lectures we will look at the physical basis of the main laser diagnostic methods using major and minor species viz. LIF, CARS, DFWM, LIGO and PS. We will then show how they are used to measure important combustion parameters such as temperature and species concentrations in one and two dimensions. Each technique will then be illustrated by applications to species and temperature measurement in flames and engines. These applications will highlight the criteria to be considered when choosing an appropriate measurement method for specific situations.

**Laser Induced Fluorescence, LIF**

When the frequency, \( \nu \), of a tunable laser, passing through an absorbing gas, is scanned, fluorescence emission may be observed when the frequency matches that of a transition in the atoms or molecules of the gas [2]. The intensity of the fluorescence is proportional to the rate of excitation to the upper state and so the LIF indicates the absorption spectrum of the medium. The LIF intensity is given by a rate equation:

\[
\frac{dn_2(t)}{dt} = n_1(t)[B_{12}I_0 + O_{12}] - n_2(t)[B_{21}I_0 + O_{21} + A_{21}]
\]
\( n_i(t) \) and \( n_j(t) \) are populations of levels 1 and 2.

\( B_{ij} \) is the Einstein coefficient for stimulated transitions between level \( i \) and \( j \).

\( I_v \) is the radiation density at frequency \( v \).

\( Q_{ij} \) is the collision induced transition rate between level \( i \) and \( j \).

\( A_{21} \) is the Einstein coefficient for spontaneous transitions from level 2 to 1.

In the steady state the rate of emission of fluorescence photons \( R_p \) is given by:

\[
R_p = n_2 A_{21} = n_i (0) B_{12} I_v \frac{A_{21}}{A_{21} + Q_{21}} \frac{1}{1 + I_v / I_{sat}}
\]

where the saturation intensity, \( I_{sat} \) is given by

\[
I_{sat} = \frac{Q_{21} + A_{21}}{B_{12} (1 + g_1 / g_2)}
\]

Low intensity: \( I_v << I_{sat} \)

\[
R_p = n_i (0) B_{12} I_v \frac{A_{21}}{A_{21} + Q_{21}}
\]

High intensity: \( I_v >> I_{sat} \)

\[
R_p = n_i (0) \frac{A_{21}}{1 + g_1 / g_2}
\]

Note that in the high intensity or saturation limit the fluorescence signal is independent of the quenching rate \( Q \). For unsaturated fluorescence the quenching rate must be determined if the signal is to be related to the absolute concentration of atoms present. \( Q \) can usually be determined.
only at low pressure (< 1 bar) where the rate is slow enough to be measured. At 1 bar the quenching rates are typically $10^{11}$ sec$^{-1}$. If $Q$ is known the absolute concentration can be determined by calibrating the detection apparatus using a known process e.g. spontaneous Raman scattering.

Since LIF depends on strong one-photon absorption it is very sensitive and may be used to detect trace species at levels of less than 1 ppm. (part per million)

2.0 Degenerate Four Wave Mixing, DFWM

In this process, three waves, having the same frequency (hence degenerate) mix via the non-linear response of a medium to produce a fourth wave [3]. Two waves interfere to “write” a stationary grating pattern or hologram and the third wave is scattered off the grating to give the signal beam. The refractive index of the medium is altered i.e. the absorption and dispersion properties are changed by partial saturation of the medium. This is a non-linear response since the change is dependent on the intensity. The non-linear susceptibility of the medium, and hence its refractive index is given by:

$$\chi(E) = -\frac{2\alpha_e}{k} \frac{(i+\delta)}{(1+\delta^2 + |E/E_s|^2)}$$

(6)
where \( \alpha_o \) is a line-centre absorption coefficient and \( k \) is the wave vector of the incident beams \( \alpha/c \), and \( \delta \) is a normalised frequency detuning of the incident light from the atomic resonance. \( E \) is the incident field intensity and \( E_s \) is the saturating field intensity:

\[
|E_s|^2 = \frac{\hbar^2}{T_1 T_2 \mu^2} = 2I_{sat} / c \varepsilon_o
\]

Where \( T_1 \) and \( T_2 \) are atomic relaxation rates for respectively the decay of the excited state population and the collision-induced polarization decay and \( \mu \) is the atomic dipole moment.

The signal is calculated by solving the wave equation using the non-linear susceptibility to describe the polarization of the medium having a length, \( L \). A strong signal is generated in a direction in which the four waves are phase matched. If the pump and probe intensities are \( I \) and \( I_{pr} \) respectively then the signal intensity \( I_{FWM} \) is found to be:

For low intensity: \( I \ll I_{sat} \)

\[
I_{FWM} = \frac{4\alpha_o^2 L^2 I^2}{(1 + \delta^2) I_{sat}^2} I_{pr}
\]

(8)

For high intensity: \( I \gg I_{sat} \)

\[
I_{FWM} = \frac{\alpha_o^2 L^2}{16(1 + \delta^2)} \frac{I_{sat}}{I} I_{pr}
\]

(9)

For saturating intensities the DFWM signal can be made insensitive to collisional quenching. \( I_{FWM} \) is proportional to \( \alpha_0 \) and hence to the square of the atomic or molecular population in the initial quantum state. Since this population depends on temperature, in Boltzmann equilibrium, the relative intensity of the DFWM spectral lines gives a measure of temperature. DFWM is used to measure temperature in flames and plasmas. Since the process is resonant for each of the interacting waves, DFWM is very sensitive and can be used to detect trace species e.g. radicals OH, C_2, at concentrations of a few ppm. [4].

3.0 Laser Induced Grating Spectroscopy, LIGS

The process of DFWM involves the modification of the material refractive index by changes in the molecular energy level populations. The incident fields alter the complex refractive
index resulting in a change in the absorption and dispersion properties of the material. Interference between one pump field and the probe field leads to a spatial variation in the refractive index in the form of a regular grating pattern. The signal arises from scattering of the second pump beam by this grating. This change in refractive index arises from the polarization induced by the interfering beams and it usually relaxes so rapidly that the signal is generated only when all three incident beams overlap in time. However, it is found that in some cases, especially at high pressures (more than one atmosphere) a signal is generated even when the third laser pulse is delayed until after the initial two pulses have interacted. Furthermore, this signal increases as the pressure of the gas is increased whereas the DFWM signal decreases rapidly with increasing pressure.

The mechanism for generating this new signal arises from the effects of molecular collisions in which some of the molecular oscillation energy is quenched i.e. some energy absorbed from the radiation field is lost in vibrational or rotational relaxation processes and does not return to the field as scattered radiation. This energy dissipation results in local heating of the medium in the regions of highest field strength and leads to a grating structure being imposed due to variation of temperature and density. The temperature grating is stationary in space but the sudden production of a density grating leads to two acoustic waves which propagate in opposite directions with a wave vector normal to the grating planes. The temperature grating decays by thermal diffusion and the acoustic waves by viscous damping processes. The exponential decay times for both the temperature and acoustic gratings increase with increasing pressure.

As the acoustic waves travel onwards they periodically interfere constructively and destructively with the stationary temperature grating leading to a periodic modulation of the grating scattering efficiency. The scattered signal will then oscillate in time with a period determined by the speed of sound in the gas. The gratings may be probed by a cw laser incident at the Bragg scattering angle, \( \phi \), appropriate for the probe laser wavelength, \( \lambda \), and grating spacing, \( d \):

\[
\lambda = 2d \sin \phi
\]  

(10)

The temporal oscillations of the signal give a measure of the local sound speed from which the temperature may be deduced. The rate of exponential decay is determined by the pressure (density) of the gas and so from a single measurement both the temperature and pressure may be derived. However, it should be noted that accurate values of temperature and pressure require detailed knowledge of the gas composition and gas dynamic properties of the constituents.
The production of these gratings may be caused by absorption and quenching processes or electrostriction effects. A class of techniques is based on these effects known as Laser Induced Thermal Grating Scattering, LITGS, or Laser Induced Thermal Acoustics, LITA, [5]. Gratings induced by electrostriction are particularly interesting as they do not require the presence of a resonantly absorbing gas species. However they do require a much more energetic laser pulse to generate a sufficiently strong LITA signal to be detected.

4.0 Coherent Anti-Stokes Raman Scattering, CARS
CARS is an example of a more general four wave mixing process [6]. Two of the three input waves have the same frequency, $\omega_p$ – the pump beams, and the third wave, $\omega_s$ – the Stokes beam, is at a frequency where the difference matches a vibration or rotational resonance, $\omega_v$ in a molecule

$$\omega_p - \omega_s = \omega_v$$

A second pump photon scatters off the induced polarization at $\omega_v$ to produce a signal at the anti-Stokes frequency:

$$2\omega_p - \omega_s = \omega_p + \omega_v = \omega_{AS}$$

The coupling of the four waves is described by a CARS susceptibility:
\[ \chi_{\text{CARS}} = \frac{\varepsilon_0 N \left( \frac{\partial \alpha}{\partial x} \right)^2}{8 m \left[ \omega^2_v - (\omega_p - \omega_s)^2 + i(\omega_p - \omega_s) \Gamma \right]} \]  

where \( \frac{\partial \alpha}{\partial x} \) is the Raman polarizability of the medium giving a measure of the variation of polarizability, \( \alpha \), as a function of displacement, \( x \), along the axis of vibration. \( \Gamma \) is the damping constant related to the spontaneous Raman linewidth of the transition. \( m \) is the nuclear mass and \( N \) is the population of the initial quantum state.

The intensity of the CARS signal is found by using \( \chi_{\text{CARS}} \) to determine the polarization in the non-linear wave equation.

\[ I_{\text{CARS}} = \frac{\omega_{AS}^2}{n_p n_s n_{AS} c^2 \varepsilon_0^2} I_p I_s |\chi_{\text{CARS}}|^2 \left[ \frac{\sin(\Delta k L/2)}{\Delta k L/2} \right]^2 \]  

The process may be considered as the writing of a grating by interference of two waves at different frequency, \( \omega_p \) and \( \omega_s \). In this case the grating is non-stationary. Scattering of a pump wave off this moving grating results in a Doppler shifted signal corresponding to the anti-Stokes signal. As in DFWM the process must be phase matched for efficient signal generation i.e. \( \Delta k = 2k_p - k_s - k_{AS} = 0 \). This is arranged by suitable alignment of the input beams.

Since the signal is proportional to \( |\chi_{\text{CARS}}|^2 \) the spectral intensity will depend on \( N \) and hence on temperature. A broadband laser may be used as the Stokes beam, \( \omega_s \), giving anti-Stokes signals from a range of initial quantum states in a single shot of the laser. Spectral analysis of the broadband CARS signal gives a single-shot measurement of gas temperature. This is widely used for temperature measurement in flames and engines.
5.0 **Polarization Spectroscopy, PS**

Polarization spectroscopy [7] uses a strong, polarized pump beam and a weak, linearly polarized probe beam, both derived from the same laser and arranged to cross at a small angle in the sample. A crossed polarizer (analyzer) is placed in the probe beam after it emerges from the sample so that no light will be transmitted to the detector. When the laser is tuned to resonance with a transition in the molecule, the pump beam selectively depopulates some of the degenerate magnetic sub-levels of the lower energy level. The induced anisotropy in the refractive index leads to a slight rotation of the probe polarization (and a slight ellipticity) resulting in a signal being transmitted by the analyzer given by:

\[
I_{\text{sig}} \propto I_{\text{las}} (\Delta \alpha L)^2 \frac{1}{(1 + x^2)}
\]

where \( L \) is the interaction length, \( x \) is the detuning \((\omega - \omega_o)/\gamma\), and \( \gamma \) is the homogeneous width, and \( \Delta \alpha \) is the difference in absorption coefficients for right and left circularly polarized light in the sample.

\[
\Delta \alpha = I_{\text{las}} \alpha_e S_o \varepsilon(J)
\]

where \( \alpha_e \) is the line centre absorption coefficient, \( \varepsilon(J) \) is a numerical factor of order unity depending on the angular momentum of the molecular level involved, \( S_o \) is the saturation parameter. We find
\[ I_{s8} \propto J_{1a8}^3 N_0^2 |\mu|^2 \varepsilon^2 (J) L^2 \frac{1}{(1 + x^2)} \]  

where \( \mu \) is the dipole moment of the transition and \( N_0 \) is the lower state population.

The numerical factors \( \varepsilon(J) \) are tabulated and take large values for R and P branch lines when the pump beam is circularly polarized and large values for Q branch lines when the pump is linearly polarized. The signal intensity \( I_{s8} \) depends on the square of the lower level population \( N_0 \) which is determined by the temperature under conditions of thermal equilibrium.

6.0 Temperature

The measurement of gas temperatures usually relies upon an assumption of thermal equilibrium i.e. the population of the molecular energy levels is in the most probable arrangement. Statistical mechanics tells us that under these conditions the population of an energy level, \( N_n \), with an energy, \( E_n \), will be given by the Boltzmann equation:

\[ N_n = N_0 \exp[-E_n/kT] \]  

where \( N_0 \) is the population in the ground state, \( k \) is Boltzmann’s constant (1.38 \times 10^{-23} \text{JK}^{-1}) and \( T \) is the temperature in degrees Kelvin. More generally we need to consider the degeneracy of the levels i.e. the number of states with the same energy. In a molecule, for rotational energy levels with an angular momentum quantum number \( J \), this is \( (2J+1) \). The rotational energy of a molecule is given by:

\[ E_i = B_v h \epsilon J(J+1) \]  

where \( B_v \) is the rotational constant which depends on the moment of inertia of the molecule, \( c \) is the speed of light and \( h \) is Planck’s constant. Thus the population of any excited level is proportional to a Boltzmann factor:

\[ N_i \sim \{(2J+1) N_0 h c/kT\} \exp[-B_v h \epsilon J(J+1)/kT] \]  

In principle any method that produces a signal proportional to the level populations \( N_i \) can be used to deduce the temperature. For example Laser Induced Fluorescence, LIF, may be used to generate a spectrum by scanning the laser frequency across the absorption lines of the molecule. The intensity of the LIF signal, \( I_{\text{LIF}} \), gives a measure of the initial level populations. Normalizing the signal to take account of the degeneracy factor \( (2J+1) \) allows us to plot a semi-logarithmic graph of \( \ln\{I_{\text{LIF}}/(2J+1)\} \) vs the rotational energy, \( B_v h \epsilon J(J+1)/kT \), yielding a slope of
Signals generated by coherent methods such as DFWM and CARS are proportional to $N^2$ and must be scaled accordingly before determining the Boltzmann plot.

The Boltzmann plotting method requires that the spectral lines be well resolved. An alternative method is to calculate a theoretical spectrum using the temperature as a variable. Overlapping of spectral features or unresolved features can be modelled and the theoretical spectrum compared to that recorded experimentally. The temperature is derived by finding the value of temperature that gives the best fit to the data. This is the basis of the widely used method of CARS thermometry but is also used for both LIF and DFWM.

A major complication in these thermometry methods arises from the effects of molecular collisions. Collisional quenching of LIF may vary within a flame depending on the species present at each location. An additional complication is that the collisional quenching rates may vary as a function of the quantum number $J$. In some cases the major quenching rates have been measured and corrections can be applied. Alternatively the signals may be made insensitive to quenching by using saturation of the transitions or pumping to pre-dissociating levels.

A simple variant of the Boltzmann method uses only two spectral lines that can be excited simultaneously by two independently tunable lasers. The temperature is then inferred directly from the ratio of the signals arising from two different initial energy levels of known energy separation. If both transition use the same upper level then the quenching effects will be the same for both spectral lines and will cancel out. However two-line methods are inherently less accurate than multi-line methods in which errors can be effectively averaged over many measurements.

### 7.0 Concentration

The concentration of combustion species is most readily measured by linear absorption and sophisticated methods using tunable diode lasers have been developed to detect concentrations as low as parts per billion. These methods are simple, accurate and reliable and give an absolute measure of the concentration. However they yield only a line-integrated measurement i.e. they measure the total number of absorbing molecules along the line of sight. LIF can yield spatial resolution by imaging the fluorescence emitted at right angles to the laser beam as it propagates through the gas. The signal can also be calibrated to allow the absolute concentration to be measured. This is illustrated by measurements in a low pressure flame or plasma.

The LIF signal is measured by using a photomultiplier system. The electrical signal recorded as a function of incident laser intensity will depend on the efficiency of the detector and the collection efficiency of the optical system. These unknown efficiencies can be calibrated by generating a signal at the same wavelength as the detected LIF signal using a known process. Spontaneous Rayleigh or spontaneous Raman scattering can be used to give a calibration signal since the scattering cross-sections for these processes are known accurately. For example the laser may be tuned to generate a spontaneous Raman signal at the LIF wavelength from a measured concentration of molecular hydrogen. The electrical signal which is proportional to the number of scattered photons is measured for a known incident laser energy (i.e. number of incident photons). The combined optical and electrical detection efficiency is then used to calculate the number of
scattering molecules from the measured number of LIF photons. Two other parameters are required before the absolute concentration of the molecules can be deduced. Firstly the temperature must be known as this determines the fraction of molecules in each quantum state and thus the number of molecules scattering at each wavelength. Secondly, the rate of quenching needs to be measured by recording the time decay of the LIF signal. At pressures of 1 bar or above the quenching times in flames will be typically less than a few nanoseconds and so picosecond techniques may be required to determine the corresponding rates.

LIF has found many applications in mapping the distribution of combustion species in flames and engines. The excitation beam is formed into a thin sheet that illuminates a plane section through the region of interest. Fluorescence emitted perpendicular to this plane — planar laser induced fluorescence, PLIF, can be readily imaged onto a 2-D detector such as a CCD camera. This technique is widely used for imaging flame fronts and turbulent flame structures. If two lines are excited simultaneously the resulting PLIF images may be used to derive a 2-D map of the temperature. Provided that any necessary quenching corrections are applied the ratio of the intensity at each point yields a two-line LIF measurement of the temperature.

2-D imaging of concentrations and temperatures can also be achieved using DFWM and PS. In this case of DFWM the reflected signal is used to form an image on a CCD camera with a spherical lens. DFWM imaging can potentially be used to image species that do not fluoresce. Several important combustion species do not yield LIF signals e.g. CH₃, HCO etc. Two line imaging can also be used to provide 2-D maps of temperature in flames using DFWM and PS.
Bibliography
The following lists some review articles and texts that provide suitable background to the material covered in these lectures:


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LASER-BASED TEMPERATURE MEASURING TECHNIQUES

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Abstract

Combustion is one of the most complicated technologies especially in turbulent medium. Combustion diagnosis requires advanced instantaneous and simultaneous measuring techniques for flow field and reactive scalar measurements. Lasers offered a unique tool for quantitative non-intrusive techniques in turbulent as well as in supersonic flames. The development of laser based techniques has achieved great success in the last thirty decade of this century. Our improved understanding of turbulent combustion is due to the developed laser techniques. In turbulent flames, the flow field affects greatly the combustion process. Information about the flow field is thus of great importance to the understanding of turbulent combustion. The flow field is often three-dimensional and can be described by velocity measurements for one and multi-components of the velocity vector, or imaging for instantaneous flow field picture.

1.0 INTRODUCTION

Laurendeau (1988) reviews laser thermometry techniques. The major techniques are Rayleigh scattering, laser induced fluorescence (LIF) and Coherent Anti-Stokes Raman Scattering (CARS). In addition, Raman scattering can also be used for temperature measurements from the total number density (Dibble et al., 1987).

2.0 RAYLEIGH SCATTERING THERMOMETRY

Rayleigh scattering is a molecular elastic process that was discovered much earlier than lasers by Lord Rayleigh (1871). The scattered Rayleigh signal is inversely proportional to temperature and directly proportional to density. The scattered Rayleigh signal is related to the type of gases in the probe volume by a parameter called Rayleigh cross-section. It is also proportional to the laser energy, solid angle of the collection optics and probe volume. The Rayleigh cross section varies inversely with the fourth power of the laser wavelength (Cottolica, et al., 1976; and Dibble and Hollenbach, 1981). The Rayleigh cross-sections for different gases can be calculated from the data in Landolt-Börstein (1962). In air with a 532 nm laser the Rayleigh scattering cross-section is about $5.99 \times 10^{-28}$ cm$^2$/sr. Long (1992) listed some Rayleigh cross-sections some important species for hydrocarbon flames. The Rayleigh signal is found to vary inversely with the third power of the laser wavelength (see Mansour 1993). This explains the blue color of the sky as mentioned earlier by Lord Rayleigh (1871) where the blue is the shortest wavelength in the visible spectrum. Based on this fact, UV lasers should provide stronger Rayleigh signal than visible lasers and, therefore are
preferred in Rayleigh thermometry. In addition for imaging purposes the laser energy per square cm in the laser sheet is weaker than in the laser beam for single point.

The Rayleigh signal is collected at 90° to the laser beam, or sheet. The collected signal by a detector (e.g. photocathode of photomultiplier, PM, tune or imaging intensifier to CCD camera) is directly proportional to the number of photon collected, \( N_p \).

As described by Einstein (see Haliday and Resnick, 1978) that the energy in a light beam travels through space in concentrated bundles, known later as "photons". The energy in this photon, \( E_p \) is defined as:

\[
E_p = h \nu
\]  
(1)

Where \( h \) is Planck's constant \( (= 6.63 \times 10^{-34} \text{ Kgm2/S}) \) and \( \nu \) is the frequency of light from

\[
\nu = c / \lambda
\]  
(2)

with \( \lambda \) the wavelength and \( c \) the speed of light \( (= 3 \times 10^8 \text{ m/s}) \). Eq. (1) can be written as:

\[
E_p = h c / \lambda
\]  
(3)

\[
E_p = \frac{1.989 \times 10^{-16}}{\lambda (\text{nm})}, \text{ Joules}
\]  
(4)

where

\[\text{leV} = 1.6 \times 10^{-19} \text{ Joules}\]

So,

\[ E_p = 1243 / \lambda (\text{nm}) \quad \text{eV} \]

The photocathode receives photons and emits photoelectrons, where the probability for emission of a photoelectron from the photocathode for each incident photon is called the quantum efficiency, \( \eta_q \). This depends on the wavelength of the collected photons. So, \( \eta_q \) is called \( \eta_q (\lambda) \).

The absolute sensitivity of the detector, \( S(\lambda, V) \), is defined as the product of its gain \( G(V) \) and the \( \eta_q (\lambda) \) as

\[ S(\lambda, V) = \eta_q (\lambda) \times G(V) \]

\( G(V) \) is used to increase the detection limit, but it does not change the signal-to-noise ratio (SNR). The SNR is ultimately limited by the number of photon collected and the quantum efficiency. Thus,
SNR = \sqrt{\eta_q (\lambda) x N p} \hspace{1cm} (5)

The photocathode is a photon counter, so the signal collected is directly proportional to the product of the total number of photon and the quantum efficiency. In Rayleigh measurements, the number of photons is proportional to the product of the total number of photons in the laser beam, \( N_{PT} \), the number density of the molecules in the measuring volume, \( N \), and the effective Rayleigh cross section as follows,

\[
N_{PT} \propto N_{PT} N \left[ \frac{d\sigma}{d\Omega} \right]_{\text{eff}}
\]

The total number of photons, \( N_{PT} \), in a laser beam with energy of \( E_1 \) is obtained from:

\[
N_{PT} = \begin{bmatrix} E_1 \\ E_P \end{bmatrix}
\]

\[
\left[ \frac{d\sigma}{d\Omega} \right]_{\text{eff}}
\]

is the effective Rayleigh cross section defined as:

\[
\left[ \frac{d\sigma}{d\Omega} \right]_{\text{eff}} = \Sigma x_i \sigma_i
\]

(7)

\( x_i \) is the species mole fraction and \( \sigma_i \) is the species Rayleigh cross section that is defined as:

\[
\sigma_i = \frac{4\pi^2 (n_{oi} - 1)^2}{N_o^2 \lambda^4} \times \frac{3}{3 - 4\rho_{vi}} \hspace{1cm} \text{cm}^2
\]

(8)

where:

- \( N_o \) : the number of molecules for an ideal gas at STP
- \( \lambda \) : ( = 2.687 \times 10 \text{ molecules/cm}^3)
- \( \rho_{vi} \) : the wavelength in \( \text{cm} \)
- \( \rho_{vi} \) : the depolarization ratio of the Rayleigh line light polarized perpendicular to the place of observation
noi : the real refractive index for a transparent gas at STP (varies with wavelength)

For an ideal gas the number density is given by:

\[ N = \frac{P A_o}{RT} \]  

(9)

Where \( P \) is the pressure, \( A_o \) is the Avogadro’s number, \( T \) is the temperature and \( R \) is the universal gas constant. For low Mach number the change of the static pressure is neglected.

Based on the above analysis, the intensity of the collected Rayleigh signal may be given as:

\[ I = k \eta_o \eta_q \Omega \frac{d\sigma}{d\Omega} \left[ \lambda^4 N \right] PT \]

(10)

Where \( k \) is a proportionality factor depends on the optical properties, \( \eta_o \) is the optical collection efficiency, and \( \Omega \) is the solid angle of collecting optics. Therefore,

\[ I = \left[ k \eta_o \eta_q \Omega \frac{PA_o}{RT} \frac{E_1}{hc} \frac{4\pi^2 (\eta_o - 1)^2}{N_o^2} x \frac{3}{3 - 4p_{vi}} \right] \frac{1}{\lambda^4 T} \]

(11)

\[ I = \left[ k \eta_o \eta_q \Omega \frac{PA_o}{RT} \frac{E_1}{hc} \frac{4\pi^2 (\eta_o - 1)^2}{N_o^2} x \frac{3}{3 - 4p_{vi}} \right] \frac{1}{\lambda^3 T} \]

(12)

This equation means that the Rayleigh signal is universally proportional to the third power of the laser wavelength. Thus UV lasers should provide stronger Rayleigh signal than visible lasers.

For the same experimental set-up and laser, the above equation can be written as:

\[ I = \left[ k \eta_o \eta_q \Omega \frac{PA_o}{RT} \frac{E_1}{hc} \frac{4\pi^2 (\eta_o - 1)^2}{N_o^2 \lambda^4} x \frac{3}{3 - 4p_{vi}} \right] \frac{1}{T} \]

(13)
It can be reduced to:

\[ I = K \left( \frac{d\sigma}{d\Omega} \right)_{\text{eff}} \frac{1}{T} \]  \hspace{1cm} (14)

In isothermal flow the signal can be used to obtain the concentration, or mixture fraction, in two stream mixing flow of different Rayleigh scattering cross-section (see Escoda and Long, 1983; and Smith et al., 1989).

In a constant cross section reacting flows, the Rayleigh signal can be used to calculate the temperature (see Dibble and Hollenback, 1981) using the following equation:

\[ I = C_R \left( \frac{1}{T} \right) \]  \hspace{1cm} (15)

where \( C_R \) is a Rayleigh calibration factor which is function of the different parameters in the square brackets of Eq. (13). The calibration factor can be obtained in air at room temperature. The Rayleigh signal is collected at 90° to the incident laser beam, or sheet.

As explained above, in Eq. (14), the temperature of the flow can be obtained if the Rayleigh cross section known or constant throughout the flow. In hydrocarbon flames, the variations of effective mixture Rayleigh cross section between the products of reaction and reactants in premixed, lean and slightly rich combustion is less than 10%. The Rayleigh cross sections of important gases in hydrocarbon combustion are listed in Table 1 at a laser wavelength of 248 nm and in Table 2 a laser wavelength of 532 nm. The values of \( n_{oi} \) and \( P_{vi} \) in Eq. (8) are obtained from Landolt-Börnstein (1962) except for the species H2O where the ratio \( \sigma_i / \sigma_{N2} \) is obtained from Muller-Dethlef and Weinberg (1979). As shown in Tables 1 and 2 the Rayleigh cross section in the UV range (at 248 nm) is higher than that in the visible range.

The effective Rayleigh cross section, \( \sigma_{\text{eff}} \), of the reactants and products of some stoichiometric mixtures of hydrocarbons are listed in Table 3. The difference between the reactants and products Rayleigh cross section reflects the expected error in the measured temperature due to this difference. If the difference is relatively high addition of low Rayleigh cross section inert gas into the reactants may reduce the difference. In open flames the difference between the reactants and the surrounding air Rayleigh cross section should also be reduced (see Mansour et al., 1992).
Table 1. Rayleigh cross section of some species at a laser wavelength of 248 nm.

<table>
<thead>
<tr>
<th>Species</th>
<th>((n_0\text{m}^{-1})\times 10^6)</th>
<th>(P_{vi}\times 100)</th>
<th>(\sigma_i\times 10^{28}\text{ cm}^2)</th>
<th>(\sigma_i/\sigma_{N_2})</th>
</tr>
</thead>
<tbody>
<tr>
<td>N(_2)</td>
<td>323.2</td>
<td>3.7</td>
<td>158.86</td>
<td>1</td>
</tr>
<tr>
<td>O(_2)</td>
<td>304.0</td>
<td>6.6</td>
<td>146.48</td>
<td>0.9222</td>
</tr>
<tr>
<td>CH(_4)</td>
<td>495.8</td>
<td>0.0</td>
<td>355.37</td>
<td>2.237</td>
</tr>
<tr>
<td>C(_2)H(_2)</td>
<td>727.93</td>
<td>4.8</td>
<td>818.31</td>
<td>5.151</td>
</tr>
<tr>
<td>C(_2)H(_4)</td>
<td>710.93</td>
<td>4.8</td>
<td>780.61</td>
<td>4.91</td>
</tr>
<tr>
<td>C(_2)H(_6)</td>
<td>879.62</td>
<td>2.4</td>
<td>1155.39</td>
<td>7.273</td>
</tr>
<tr>
<td>C(_2)H(_8)</td>
<td>863.06</td>
<td>0.8</td>
<td>1088.33</td>
<td>6.851</td>
</tr>
<tr>
<td>C(_2)H(_6)</td>
<td>1239.3</td>
<td>1.0</td>
<td>2249.98</td>
<td>14.16</td>
</tr>
<tr>
<td>C(_3)H(_8)</td>
<td>155.7</td>
<td>0.9</td>
<td>35.46</td>
<td>0.233</td>
</tr>
<tr>
<td>H(_2)</td>
<td>492.1</td>
<td>7.3</td>
<td>387.81</td>
<td>2.44</td>
</tr>
<tr>
<td>H(_2)O</td>
<td>380.6</td>
<td>1.7</td>
<td>214.22</td>
<td>1.349</td>
</tr>
<tr>
<td>CO(_2)</td>
<td>319.2</td>
<td>4.15</td>
<td>155.89</td>
<td>0.981</td>
</tr>
<tr>
<td>CO</td>
<td>36.03</td>
<td>2.5</td>
<td>1941</td>
<td>0.0122</td>
</tr>
<tr>
<td>Air (dry)</td>
<td>68</td>
<td>0.9</td>
<td>6.765</td>
<td>0.0426</td>
</tr>
<tr>
<td>He</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ne</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ar</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 2. Rayleigh cross section of some species at a laser wavelength of 532 nm

<table>
<thead>
<tr>
<th>Species</th>
<th>((n_0\text{m}^{-1})\times 10^6)</th>
<th>(P_{vi}\times 100)</th>
<th>(\sigma_i\times 10^{28}\text{ cm}^2)</th>
<th>(\sigma_i/\sigma_{N_2})</th>
</tr>
</thead>
<tbody>
<tr>
<td>N(_2)</td>
<td>301.2</td>
<td>0.28</td>
<td>6.21</td>
<td>1</td>
</tr>
<tr>
<td>O(_2)</td>
<td>273.9</td>
<td>0.75</td>
<td>5.16</td>
<td>0.832</td>
</tr>
<tr>
<td>CH(_4)</td>
<td>44.6</td>
<td>0.0</td>
<td>13.605</td>
<td>2.19</td>
</tr>
<tr>
<td>C(_3)H(_8)</td>
<td>1103.97</td>
<td>1.00.24</td>
<td>84.32</td>
<td>13.58</td>
</tr>
<tr>
<td>H(_2)</td>
<td>140.5</td>
<td>0.4</td>
<td>1.351</td>
<td>0.217</td>
</tr>
<tr>
<td>H(_2)O</td>
<td>254.6</td>
<td>0.99</td>
<td>4.445</td>
<td>0.716</td>
</tr>
<tr>
<td>CO(_2)</td>
<td>453.6</td>
<td>0.15</td>
<td>14.22</td>
<td>2.229</td>
</tr>
<tr>
<td>CO</td>
<td>336.9</td>
<td></td>
<td>7.75</td>
<td>1.249</td>
</tr>
</tbody>
</table>
Rayleigh thermometry has proved success because the signal is quite strong and linearly proportions with temperature. Single point (see Masri et al., 1988a, 1988b, 1988c; Dibble and Hollenbach, 1981; and Mansour et al., 1991), two-dimensional (O'Young and Bilger, 1996; Komiyama et al., 1996, and Long, M.B., 1992) and three-dimensional measurements (Mansour 1993; and Mansour et al., 1992) were obtained in turbulent flames. These data were used to calculate the thickness of the reaction zone, 3-D gradients, scalar dissipation rate and even velocity.

### Table 3 Rayleigh cross sections of the reactants and products of stoichiometric flames of some fuels

<table>
<thead>
<tr>
<th>Reactants</th>
<th>(x_i) Mole Fraction</th>
<th>(\sigma_j/\sigma_{N_2})</th>
<th>Products</th>
<th>(x_i) Mole Fraction</th>
<th>(\sigma_j/\sigma_{N_2})</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\text{CH}_4)</td>
<td>0.095</td>
<td>2.19, 2.287</td>
<td>(\text{CO}_2)</td>
<td>0.095</td>
<td>2.29</td>
</tr>
<tr>
<td>(\text{O}_2)</td>
<td>0.19</td>
<td>0.809, 0.832</td>
<td>(\text{H}_2\text{O})</td>
<td>0.19</td>
<td>0.716</td>
</tr>
<tr>
<td>(\text{N}_2)</td>
<td>0.715</td>
<td>1.0</td>
<td>(\text{N}_2)</td>
<td>0.715</td>
<td>1.0</td>
</tr>
<tr>
<td>(\sigma_{\text{eff}} = \sum x_i \sigma_j/\sigma_{N_2})</td>
<td>1.077</td>
<td></td>
<td>(\sigma_{\text{eff}} = \sum x_i \sigma_j/\sigma_{N_2})</td>
<td>1.069</td>
<td></td>
</tr>
</tbody>
</table>

#### (b) Propane

<table>
<thead>
<tr>
<th>Reactants</th>
<th>(x_i) Mole Fraction</th>
<th>(\sigma_j/\sigma_{N_2})</th>
<th>Products</th>
<th>(x_i) Mole Fraction</th>
<th>(\sigma_j/\sigma_{N_2})</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\text{C}_3\text{H}_8)</td>
<td>0.0403</td>
<td>14.1</td>
<td>(\text{CO}_2)</td>
<td>0.116</td>
<td>2.29</td>
</tr>
<tr>
<td>(\text{O}_2)</td>
<td>0.2015</td>
<td>0.809, 0.832</td>
<td>(\text{H}_2\text{O})</td>
<td>0.155</td>
<td>0.716</td>
</tr>
<tr>
<td>(\text{N}_2)</td>
<td>0.758</td>
<td>1.0</td>
<td>(\text{N}_2)</td>
<td>0.729</td>
<td>1.0</td>
</tr>
<tr>
<td>(\sigma_{\text{eff}} = \sum x_i \sigma_j/\sigma_{N_2})</td>
<td>1.489</td>
<td></td>
<td>(\sigma_{\text{eff}} = \sum x_i \sigma_j/\sigma_{N_2})</td>
<td>1.106</td>
<td></td>
</tr>
</tbody>
</table>
(c) Hydrogen

<table>
<thead>
<tr>
<th>Reactants</th>
<th>Products</th>
</tr>
</thead>
<tbody>
<tr>
<td>Species</td>
<td>(x_i) Mole Fraction</td>
</tr>
<tr>
<td>___</td>
<td>___</td>
</tr>
<tr>
<td>( \text{H}_2 )</td>
<td>0.296</td>
</tr>
<tr>
<td>( \text{O}_2 )</td>
<td>0.148</td>
</tr>
<tr>
<td>( \text{N}_2 )</td>
<td>0.556</td>
</tr>
</tbody>
</table>

The application of this technique is limited to dust free environment in order to avoid Lorenze-Mie scattering which is about three orders of magnitude higher than Rayleigh scattering signal at higher wavelengths. The optical arrangement of this technique is quite simple with a laser, focusing lens, and interference filter, and a signal detector (e.g. PM tube or CCD camera), as shown in Fig. 1. It is thus the most commonly used techniques in temperature measurements. a combination with Raman diagnostics has achieved very much success.

The combination of Raman and Rayleigh techniques is possible since both require one laser beam. This combination provides very essential data about major species mass fraction and temperature (Dibble et al., 1987). This technique was a very successful technique in turbulent clean flames of hydrogen and hydrocarbon flames (Masri et al., 1988a, 1988b, 1988c; Mansour et al., 1990, 1991; and Starner et al., 1990a, 1990b). The relatively simple optical system has attracted many research groups to apply similar techniques either for single point measurements or recently for one-dimensional measurements using tunable UV Excimer laser (see Mansour and Chen, 1996).
Fig. 1 A schematic diagram of Rayleigh optical arrangement
3.0 CARS THERMOMETRY

CARS thermometry can be obtained from the analysis of the CARS signal, as described in another lecture in this course, of any species in the measuring volume, e.g. N$_2$. The rotational-vibrational population of the Raman transitions of the probed species varies with temperature as shown by Palmer (1989) in Fig. 2 for N$_2$. The existence of nitrogen in almost all combustion systems and the sensitivity of its Q-branch spectrum to temperature, as shown in Fig. 2 have made it a preferable species for CARS thermometry.

The temperature can be obtained by fitting the recorded signal from N$_2$ with its calculated spectrum using the least square fit method, see Fig. 2. Thus the CARS measured temperature is the spectroscopic temperature that is, in most combustion situations, equal to the transitional temperature. In some applications, e.g. plasmas, this equation is not true (Nibier et al., 1976; Shaub et al., 1977; Pealat, et al., 1981; Taran, 1987, and Yancey et al., 1987). The error in the calculated temperature from a single shot CARS is about ± 50 K while for multi shots it is about 1 % of the mean. Other species have also been used for CARS thermometry, e.g. H$_2$, H$_2$O and CO$_2$. The variation of H$_2$O spectrum with temperature is quite complicated (Hall, 1979). On the other hand, the application of H$_2$ CARS thermometry in H$_2$-air flames (Shirley et al. 1979) was quite successful because H$_2$ has a large Raman scattering cross-section, i.e. stronger signal, and the separation between the rotational lines is wide and hence interference from non-resonant susceptibility is minimized.

![Figure 2: Variation of CARS N2 spectrum as a function of temperature from 300 to 2300 K (Palmer, 1989)]
**Fig. 3 General Approaches to LIF Thermometry (Eckbreth, 1988)**

## 4.0 LIF AND LIPF THERMOMETRY

The laser induced fluorescence technique, described above, can be used for temperature measurements. It depends on measuring the distribution of population over two or more states, in vibrational rational states. LIF is used for radicals which occur at high temperature in the flame and, hence, high temperature in the flame and, hence, high temperatures can only be measured. For molecular LIF detecting, e.g. NO (McKenzie and Gross, 1981) or O2 (Massey and Lemon, 1984), a wide range of temperature can be measured. However, Rayleigh thermometry is more simple for application than CARS and LIF thermometry techniques.

LIF thermometry can be done with three approaches, excitation scans (see summary of Anderson et al., 1982), two-line approaches (Haraguchi et al., 1977; and Cattolica, 1981) or thermally assisted techniques (Crosley and Smith, 1980; Chan and Daly, 1980; and Zizak et al., 1981). Eckbreth (1988), Fig. 3, describes these approaches. The most often employed approach is the excitation scans in steady-state flames where there is enough time for excitation scan over the vibration rotational ground electronic state. Excitation with one laser at wavelength λ of the molecule from the ground followed by emission, fluorescence, to the ground state. Scanning and analyzing the signal leads to evaluate temperature. In this approach, analyzing the collected spectrum at the ground state, as shown in Fig. 3, is similar to CARS signal analysis special considerations in the collection optics, e.g. wide detection band pass, are necessary to obtain the correct temperature (Crosley and Smith, 1980).

The two-line approach needs two lasers as shown in Fig. 3. The method is sequential, i.e. excitation first from level 1 to level 3 and the fluorescence from level 3 to level 2 is collected, then excitation from level 2 to level 3 and the fluorescence from level 3 to level 1 is collected. From these two collected spectra, the population difference can be calculated and then the temperature can be evaluated by
Boltzmann expression. Using two lasers adds more difficulties to the technique. The third approach is shown in Fig. 3. It needs continuous tuned laser (Eckbreth, 1988).

The LIPF thermometry is described in another lecture in this course with LIP scattering from species measurements. It has the advantages of being independent of quenching problems that are very dominant in LIF measurements. Quenching in LIF measurements is even too intense in high-pressure combustion environment.
LASER-BASED SPECIES CONCENTRATION AND DENSITY MEASURING TECHNIQUES

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ABSTRACT

Measurements of instantaneous and simultaneous species concentration, major, intermediate and radicals, provide useful data for studying the chemistry of the flame. In addition to the flow field information and temperature, a full description of the flame structure may be possible. Laser-based techniques for scalar measurements are based on different phenomenon as laser interacts with matter. The most known phenomena are elastic scattering, inelastic scattering, laser absorption and fluorescence. Each of these phenomena are related to the status and concentration of the gaseous molecules within the measuring volume. Temperature and major and minor species concentration measurements techniques have been developed based on these phenomena.

INTRODUCTION

Measurements of instantaneous and simultaneous species concentration, major, intermediate and radicals, provide useful data for studying the chemistry of the flame. In addition to the flow field information and temperature, a full description of the flame structure may be possible. In this lecture the major techniques used for species concentration measurements are described. The application of each of the following techniques depends on the concentration level of the measured species. The scattering techniques for species measurements may be Fluorescence, Rayleigh scattering, Coherent Anti-Stokes Raman and then Raman scattering. Lorenz-Mie is considered the strongest because it is a particle scattering technique and not a molecular scattering.

RAMAN SCATTERING

Introduction

The Raman scattering is a molecular inelastic scattering that has been formulated by Raman (1928). In this technique when a laser excites a molecule, inelastic scattering of light from the molecule occurs; i.e. scattering at shifted wavelength from the incident beam. The Raman scattering is termed rotational, vibrational or electronic (Long, 1977) depending on the nature of the energy change between the molecules and incident laser quanta. The scattering occurs simultaneously, within picoseconds, from all molecules in the measuring volume. Raman scattering is incoherent light scattering process that is shown in Fig. 1 Raman shift occurs at higher frequency (Anti-Stokes) and at lower frequency (Stokes), as illustrated in Fig. 1.
The main advantage of Raman scattering are:
- No laser tuning is required
- Only one laser is required to monitor all the species in the measuring volume.
- The Raman signal is not subjected to quenching
- Calibration is possible
- Accurate measurements are quite feasible for major combustion species.

The disadvantages are:
- The Raman signal is very weak
- The Raman signal is subjected to some interference, e.g. LIF and Raman lines cross talk
- The Raman signal is affected by the presence of particles or high luminosity in the flame.

Rayleigh scattering, at the same laser frequency, occurs simultaneously with Raman scattering, as shown in Fig. 1. This is another advantage to combine both Raman and Rayleigh in one technique, this provides both temperature and species concentration simultaneously.

![Diagram of Raman and Rayleigh scattering](image)

**Fig. 1 Raman and Rayleigh light scattering process and spectra**

**Vibrational Raman Technique**

The vibrational Raman scattering signal is related to the species number density in the measuring volume by (see Dibble et al. 1987)
When \( N_s \) is the species number density, \( \sigma_R \) is the species Raman cross-section, \( E_l \) is the laser energy; \( L \) is a probe dimension; \( \Omega \) is the collection solid angle and \( \eta \) is the collection optics efficiency. The Raman cross section varies inversely with the fourth power of the laser wavelength. The Raman cross-section is much weaker than Rayleigh cross-section (around \( 10^{-31} \text{ cm}^2/\text{sr} \) for Raman and \( 10^{-28} \text{ cm}^2/\text{sr} \) for Rayleigh). This leads to very weak collected Raman signal, about \( 10^{-14} \) of the incident laser energy. Eckbreth (1988) presents in his book a list of Raman cross section of some species as shown in Table 1.

\[
I_{Ran} = E_l N_s \sigma_R L \eta \Omega
\]  

(1)

<table>
<thead>
<tr>
<th>Species</th>
<th>Vibrational Frequency (cm(^{-1}))</th>
<th>Vibrational</th>
<th>Cross</th>
<th>Sections</th>
<th>Rotational ( \sigma_{ss}(J'' \rightarrow J') )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( N_2 )</td>
<td>2330.7</td>
<td>3.5</td>
<td>0.68</td>
<td>0.46</td>
<td>5.4(6(\rightarrow)8)</td>
</tr>
<tr>
<td>( H_2 )</td>
<td>4160.2</td>
<td>8.7</td>
<td>1.32</td>
<td>0.88(Q)</td>
<td>0.37(Q)</td>
</tr>
<tr>
<td>( O_2 )</td>
<td>1556</td>
<td>4.6</td>
<td>0.72</td>
<td>0.65</td>
<td>1.0(1(\rightarrow)0)</td>
</tr>
<tr>
<td>( NO )</td>
<td>1877</td>
<td>1.5</td>
<td>0.15</td>
<td>0.2</td>
<td></td>
</tr>
<tr>
<td>( NO_2 )</td>
<td>1320</td>
<td>51.0</td>
<td></td>
<td>7.37</td>
<td></td>
</tr>
<tr>
<td>( NH_3 )</td>
<td>3334</td>
<td>11.0</td>
<td>2.75</td>
<td>1.3</td>
<td></td>
</tr>
<tr>
<td>( CO )</td>
<td>2145</td>
<td>3.6</td>
<td></td>
<td>0.48</td>
<td>0.27</td>
</tr>
<tr>
<td>( CO_2 )</td>
<td>1388</td>
<td>4.2</td>
<td>0.77</td>
<td>0.6</td>
<td>53.0</td>
</tr>
<tr>
<td>( CH_4 )</td>
<td>2915</td>
<td>21.0</td>
<td>3.3</td>
<td>2.6</td>
<td></td>
</tr>
<tr>
<td>( C_2H_4 )</td>
<td>3020</td>
<td>16.0(Q)</td>
<td></td>
<td>1.9</td>
<td></td>
</tr>
<tr>
<td>( C_2H_6 )</td>
<td>993</td>
<td></td>
<td></td>
<td>0.88</td>
<td></td>
</tr>
<tr>
<td>( C_6H_6 )</td>
<td>3070</td>
<td>30.0</td>
<td>3.8</td>
<td>3.7</td>
<td></td>
</tr>
<tr>
<td>( V_1 )</td>
<td>991</td>
<td>44.0</td>
<td>5.0</td>
<td>5.6</td>
<td></td>
</tr>
</tbody>
</table>

(UNITS OF 10-30 cm\(^2\)/sr)
Equation (1) can be reduced to

\[ N_i = C_i(T)I_{RAM} \]

(2)

where, \( C_i(T) \) is a temperature dependent calibration factor which includes all parameters in Eq. (1) and ultimately obtained by calibration in cold and hot gases. The Raman shift and spectra depend on the molecular characteristics. Thus, the Raman signal, spectrum, can be used to measure species concentration. The variation of the Raman shift with laser wavelength is shown by Dibble et al. (1987) as shown in Fig. 2. The absorption lines of \( C_i \) are also illustrated, which indicates the interference with the Raman lines.

![Diagram showing Raman lines and laser wavelength with absorption lines of \( C_i \)]

Fig 2. The variation of Raman lines wavelength of some species (Dible et al., 1987)

The Raman spectrum for species is temperature dependent and it is usually broader at higher temperature. An example of the effect of temperature on the Raman spectrum of Nitrogen is shown in Fig. 3 (Eckbreth, 1988). The broadening of the Raman lines at high temperature should be considered in the calibration system for flame measurements.
Fig 3. The variation of N2 vibrational Q-branch Raman spectrum temperature at constant density (Eckbreth, 1988)
The Raman signal is usually collected at 90° to the incident laser beam. Since the Raman signal scatters at 4π steradians a higher f/number collection optical arrangement is recommended. A possible set-up for a Raman technique is illustrated in Fig. 4 below.

![Fig. 4 A schematic diagram of a Raman technique](image)

The collected vibrational Raman signal is spectrally dispersed using a spectrometer and then the output spectrum is recorded using a multi-channel detector or Photo-Multiplier (PM) tubes. Powerful lasers are required for Raman measurements in flames. The spontaneous Raman technique was successfully applied in turbulent diffusion flames together with Rayleigh scattering, for temperature, by Dibble et al. (1987) using a flash lamp pumped dye laser in the visible regime. A series of successful measurements based on this technique are now available (Masri et al., 1988a, 1988b, 1988c, 1990). Raman scattering has also been applied in clean flames (Lapp and Penney, 1974, Eckbreth, 1981; and Mansour et al., 1989).

The vibrational Raman scattering offers many advantages as compared to other laser-based techniques. First, the relatively simple set-up for multi-species concentration using one laser beam. Second the linear relation between the species number density and Raman signal. Third, it is not limited to the laser wavelength since a fixed Raman shift is a molecular characteristic.

These advantages made the spontaneous Raman technique a powerful tool in laser-based techniques. The Raman theory is described in details in Long (1977), Weber (1979) and Eckbreth (1988).
As described above, the Raman cross-section is inversely proportional to the fourth power of the laser wavelength. So, the application of UV lasers instead of visible lasers in Raman scattering has attracted recently some research groups. The first application of UV Raman scattering is due to Pitz and his co-workers (Pitz et al. 1990; Wehrmeyer et al., 1992; and Cheng et al. 1992). The technique is then developed from single-point measuring technique to one-dimensional measuring technique. This allows for the first time to measure the radial component of the scalar dissipation rate in turbulent flames (Reckers et al., 1993; Nandula et al., 1994a; 1994b; Grunsefeld et al., 1994; Brockhinke et al., 1995; and Mansour and Chen, 1996) is shown in Fig. 5. The scattered Raman spectrum is collected through a spectrograph and is vertically dispersed. The images collected at the exit plane of the spectrograph represent the spectrum of the major species in the measuring volume along the radial direction of the flame that is crossing the reaction zone.
5.0 Methods to Enhance the Raman Signal

The Raman signal is very weak, as described above, and thus the following methods may be recommended to enhance its intensity. There are however some limitations for each case.

1. Use high power lasers. This is limited by the gas breakdown.
2. UV lasers may be recommended, since the signal is inversely proportional with the fourth power of the laser wavelength. This limited to stoichiometric and lean flames due to the interference from poly-aromatic hydrocarbon fluorescence.
3. Use multipass optics approach for the laser beam, as shown in Fig. 6 (Eckbreth, 1988). This is limited to low-turbulent flames where large variation in the medium refractive index is not recommend.
4. Use a spherical mirror behind the focal point of the collection optics to reflect the scattered Raman signal into the collection detector.
Fig. 6 Multipass Optics for Raman Signal Enhancement

5.1 Calibration and Interference Correction

The Raman spectrum is affected by temperature, as shown above, and thus temperature dependent calibration factor is required. This can be achieved by recording the Raman spectrum of different species at different temperature levels and then include the temperature effect. In addition the Raman lines cross talk that causes interference to the Raman signals should be corrected. The cross talk can be obtained from the recorded calibration spectrum at different temperatures, this leads to temperature dependent correction parameters.

In order to test the calibration system, a calibration burner with very well known boundary conditions should be applied and tested.

Another Raman scattering process occurs if the laser wavelength is tuned near an electronic resonance of the molecule being probed. This is called near-resonant fluorescence which enhance the Raman cross-section by orders of magnitudes (Szymanski, 1967). Tuning the
laser will, however, diminish most of the enhancement achieved. This technique has not been applied successfully in flames.

6.0 LASER INDUCED FLUORESCENCE

Laser induced fluorescence (LIF) is an inelastic process. In this technique the probed molecule, or atom, is excited by the laser to a higher energy level, by photon absorption, and then followed by spontaneous emission of light. The emission may occur at a shifted wavelength from the incident laser wavelength, called fluorescence, or at the same wavelength, called resonance fluorescence. The LIF signal has a cross-section many orders of magnitude than Raman. It is suitable for intermediate species and radicals with concentration as slow as 1 ppm. (Crosley, 1980, 1981, and Crosley and Smith, 1983). The LIF scattering process is illustrated in Fig. 7, and described in details in Eckbreth (1988). The laser is tuned to a specific absorption band at the lower electronic state and then absorption occurs to move the molecule to a higher excited electronic state. This is then followed by spontaneous emission to the lower electronic state with certain fluorescence spectra.

![Fluorescence Spectrum and Excitation Scan](image)

Fig. 7. A schematic of potential energy curves for the lower and upper electronic states with vibrational (heavy) and rotational (light) energy levels (Eckbreth, 1988)

The fluorescence lifetime is between $10^{-10}$ and $10^{-5}$ sec. Within this lifetime other processes may occur and then emission may not be produced. These processes may occur and then emission may not be produced. These processes are termed under quenching (energy loss) and may be listed as dissociation, chemical reaction and energy transfer to internal energy within the molecule. This represents the major problem in LIF quantitative measurements. Correction due quenching effects requires full information about the environment, species concentrations, within the measuring volume. Many research groups have applied different approaches to estimate the errors due to quenching effects. Saturation fluorescence is one of the most appreciated approaches (Piepmeier, 1972 and Daily, 1977). In this approach the laser
intensity is made too high so that the rates of absorption and stimulated emission are much greater than the quenching rate. Thus quenching can be neglected. For some species intense unable laser is not yet available for saturation fluorescence. Some analytical models have been employed to obtain the species concentration from the analysis of the fluorescence signal (Baronavski and McDonald, 1977; Verdieck and Bonczyk, 1981 and Mailander, 1978).

7.0 LASER INDUCED PREDISSOCIATION FLUORESCENCE

The quenching problem in LIF signal is, as explained above, due to the lifetime of the LIF signal within which another possible sources of energy losses may participate and cause no LIF signal. The laser-induced predissociation fluorescence is fast and its time scale is three orders of magnitude shorter than LIF signal. The fluorescence signal is inversely proportional to the sum of the time scales of the LIF signal, quenching and the predissociation signal. Thus the predissociation time scale should dominates the collected signal and thus no quench is possible. The pioneering work in this technique is due to Andreason and his co-workers (Andreason et al. 1988, Andreason et al. 1990). Full description about LIPF spectroscopy is shown in Fig. 8. In this spectroscopy (Andreason et al. 1990), a laser beam excites a molecule from \( v''=0 \) at state 1 to \( v' = 3 \) at state 2. If the excitation from \( v'' = 0 \) at state 1 to \( v' = 0 \) at state 2, for example, fluorescence, \( f_i \) and quenching may only occur, but the excitation shown in Fig. 8 adds a pridissociation term through the curve crossing with rate \( P \). If the fluorescence and quench rates are \( F \) and \( Q \), the intensity of the collected fluorescence signal, \( I_F \), is related to the measured species number density, \( N_i \), as

\[
I_F = N_i C_i \left[ \frac{F}{(F + P + Q)} \right]
\]

Since \( P \) is much greater than \( Q \), quenching effects on the LIPF signal can be neglected. Thus the number density may be approximated as \( I_F (P/Q) \) which is independent of quenching effect.

LIPF can also be used for temperature measurements by measuring two states \( N_1 \) and \( N_2 \) with and their known energies \( E_1 \) and \( E_2 \). Then the temperature is calculated, from the arhenous relation \( N_i = g_i \exp(-E_i/kT) \), as

\[
T = \left[ \frac{(E_1 - E_2)/k}{\ln\left(\frac{N_2}{N_1}\right)} \right]^{1/2} \left( \frac{g_1/g_2}{N_1/N_2} \right)
\]

The LIPF has been applied for OH radical concentration measurements using a UV KrF excimer laser at 248 nm. One-dimensional (Mansour and Chen, 1996) and two dimensional (Anderson et al. 1990) measurements of OH have been obtained successfully in turbulent flames and in engines at high pressures.
Figure 8. LIPF spectroscopy. The potential energy curves with upper and lower electronic states.

8.6 CARS FOR SPECIES CONCENTRATION

Coherent anti-stokes Raman diagnostic is a non-linear wave mixing process. In this technique, a laser beam at frequency $\omega_1$ (pump) is combined with another laser beam at $\omega_2$ (Stokes) via a third order susceptibility of a molecule in the measuring volume. This induces a polarization which forms a third coherent beam at a third frequency $\omega_3$ that equals $(2\omega_2 - \omega_1)$. So two lasers are required for this technique. A schematic diagram of one possible optical arrangement of CARS technique, called collinear CARS, is shown in Fig. 9 below. In order to measure any of the species in the probe volume, as will be discussed later, the frequency difference between the pump beam and the Stokes one ($\omega_1 - \omega_2$) should be tuned to its Raman allowed transition. Then the CARS signal, $\omega_3$, is resonantly enhanced. This CARS signal at $\omega_3$ is a laser-like signal, which has a direction, and then a high percentage of the signal can be collected. Thus it can be discriminated against background. It is also strong in comparison to spontaneous Raman signal, explained later. In CARS the collection is highly efficient (one photon in 10,000 is produced in the CARS signal) while the Raman collection efficiency is much weaker (one photon in 10 million is produced) because its signal is distributed over a 4 $\pi$ steradian.

CARS techniques can be used for species and temperature measurements. In this section, CARS technique for species measurements is explained and CARS thermometry is explained in another lecture in this course. Since CARS is a wave mixing process a one signal can only be obtained from the two beams, $\omega_1$ and $\omega_2$. The coherent signal, $\omega_3$, is to a certain species. For more species measurements at the same time, several beams should be included. This adds more difficulties to the optical arrangement and data analysis. The theory of CARS diagnostics is described in details in Eckbreth (1984), Greenhalgh (1988) and Hall and Eckbreth (1984). The pioneering application of CARS diagnostics in combustion is due to Taran and his co-workers (Regnier and Taran, 1973; Regnier et al., 1973; Moya et al., 1975, 1977, and Peñal et al., 1980). Goss (1993) has recently reviewed CARS technology and its applications in combustion.
9.0 LASER-INDUCED INCANDESCENCE, LII, TECHNIQUE FOR SOOT MEASUREMENTS

9.1 Introduction

Eckbreth (1976) has discovered laser-induced soot incandescence (LII) as a source of interference in weak Raman measurements. It has been further investigated in more details (Eckbreth, 1977a, 1977b). This represents an error in some weakly scattering technique, e.g. Raman, where the LII signal is broad. LII signal is produced when soot particles absorb the energy provided by the laser and heated to high temperatures. At this stage the heated soot particles emit increased quantity of blackbody radiation.

More work has been carried out in the last few years to interpret the LII signal soot volume fraction measurements (e.g. Vander Wal and Weiland, 1994, Vander Wal and Dietrich 1995; Cigoli et al., 1994; Shaddix et al., 1994 and Ni et al., 1995). Time resolved LII technique has been developed recently by Will et al. (1995, 1996).

9.2 Theory
The LII signal from soot particles in the flames is related to laser absorption, heat transfer to the surrounding medium, vaporization of soot particles, thermal radiation and rise of internal energy (Will et
The basic idea is to increase soot particles temperature above the vaporization temperature by high laser energy (Will et al. 1996). Based on the conservation of energy, as shown in Fig. 10, the differential equation of temperature of spherical particles of diameter \( d_p \) is

\[
Q_{abs} \frac{\pi d_p^2}{4} E_i - \Lambda (T - T_0) \frac{\pi d_p^2}{M} \frac{\Delta H_v}{\Delta t} - \varepsilon(T) \sigma_{SB} T^4 \frac{\pi d_p^2}{6} \rho C \frac{dT}{dt} = 0
\]

The first term represents the laser energy absorbed by the soot particle, \( Q_{abs} \) is the absorption efficiency, and \( E_i \) is the irradiant energy. The second term represents the heat transfer of the soot particle at temperature \( T \) to the surroundings at \( T_0 \), \( \Lambda \) is the heat transfer coefficient. The third term represents the heat of vaporization of the soot particle, \( \Delta H_v \) is the heat of vaporization, \( M \) is the carbon molar mass and \( dm/dt \) is the rate of mass decrease. The fourth term is the thermal radiation, \( \varepsilon \) is the mean emission, and \( \sigma_{SB} \) is Stefan-Boltzmann constant. The last term is the change of the particle internal energy, \( \rho \) is the density and \( C \) is the specific heat.

**Fig. 10** Energy conservation for an excited soot particle by laser energy.
The detected signal $S$, for a given wavelength, $\lambda$, is given by (Melton, 1984 and Will et al. 1996).

$$S \propto N_r^x, \quad x = 3 + 154 \text{nm}/\lambda \quad (6)$$

10.0 ABSORPTION TECHNIQUES FOR SPECIES CONCENTRATION MEASUREMENTS

Absorption by molecules of the incident laser energy of tunable lasers can be used for species concentration measurements. LIF technique may be listed as an absorption technique. It has been used in combustion before the invention of lasers using other light sources, e.g. arc lamps, (Penner, 1959; and Gaydon, 1974). Line-center techniques in flames (Sulzman et al., 1973) or in atmosphere (Byer, 1975) have been used with success. Eckbreth (1988) describes the basis of absorption techniques in flames.

11.0 CONCENTRATION AND DENSITY MEASURING TECHNIQUES

For mixing studies of isothermal flows, Rayleigh technique or Lorenz-Mie technique can be used. Rayleigh scattering is described in another lecture in this course where the Rayleigh signal, as a molecular elastic scattering signal, varies inversely with temperature and directly with density. So, for two stream mixing process, Rayleigh scattering can be applied. Lorenz-Mie scattering, as a particle elastic scattering (see Hulst, 1957, Kerker, 1969 and Fiedlander, 1977), can also be applied. So, in order to measure concentration of one stream in two stream mixing process or the concentration in flames, one stream should be seeded with particles of small size, about one micron, and the Lorenz-Mie signal can be used to calculate the concentration. Lorenz-Mie signal is about three orders of magnitude stronger than Rayleigh. So, its application needs less powerful lasers. On the other hand, reliable mean measurements can only be obtained based on Lorenz-Mie scattering. Errors of about 200% on the rms were observed by Mansour et al. (1989a) as compared to Rayleigh measurements.

12.0 DEGENERATE FOUR-WAVE MIXING (DFWM)

12.1 Introduction

DFWM is based on the interaction of three input beams of identical frequency, $\omega$, with nonlinear medium to produce a fourth coherent signal (Rakestraw et al., 1990). The process has been described as (Rakestraw et al., 1990) the interference between the three beams given rise to an optical fringe-pattern at which the intensity of light various sinusoidally in the overlapping region, this leads to form a Bragg grating that results in the scattering of the pump beam. The beams' arrangement for DFWM is shown in Fig. 11. The unfocused beam from the laser at a specific wavelength is divided using two beam splitters to form three beams. Two beams counter propagate, called forward pump and backward pump, and the third beam, called the probe, intersects both pump beams at small angle. Thus the scattered signal beam is produced and counter and counter propagates collinear with the probe beam.
Fig. 11 A schematic diagram of the DFWM beams' arrangement

The scattered DFWM signal intensity, $I_S$, is proportional to the square number density of the sampled species, $N$, and may be written as:

$$I_S \propto B_{ij}^2 N^2 L^2 I_f I_b I_p$$  \hspace{1cm} (6)

where, $B_{ij}^2$ is the one photon line strength of the molecular transition, $L$ is the interaction length, $I_f$ is the intensity of the forward beam $I_b$ is the intensity of the backward beam and $I_p$ is the intensity of the pump beam.

The advantages of DFWM techniques are:
1. Only single laser is required
2. DFWM technique operates at low laser intensity
3. DFWM provides relatively strong signal intensity and is thus sensitive to small concentration measurement, e.g. radicals
4. Simple data analysis.

The main disadvantages are:
1. Spatial resolution is relatively poor and the application of DFWM technique to resolve thin flame structure is quite difficult.
2. Beam steering in turbulent flames causes problems in DFWM technique.

Cole et al. (1992) have applied DFWM technique for NO$_2$ and soot concentration measurements in the exhaust of a jet engine. They found that the DFWM signal intensity is proportional to NO$_2$ concentration, $N_{NO2}$, and soot concentration, $N_{soot}$, as follows:

$$I_0 \propto N^{1.9}_{NO2}$$  \hspace{1cm} (7)

$$I_0 \propto N^{1.8}_{soot}$$  \hspace{1cm} (8)

The deviation of the theoretical square dependence of the signal and measured value was explained to be due to absorption of the signal through the measured gases.

Rakestraw et al. (1990) have used DFWM technique to measure NH radical in flames. Dreier and Rakestraw (1990) have also applied DFWM technique for OH and NH radicals’ measurement in flames. In addition rotational temperature has been obtained from DFWM spectra (Dreier and Rakestraw, 1990a, 1990b). tunable laser radiation is generated at 307 nm and 335 nm for OH and NH excitation, respectively. Ewart and O’Leary (1986) and Brown et al. (1992) have also detected OH radical using DFWM techniques.

DFWM technique has been developed for imaging of atomic distribution in flames by Ewart et al. (1989). They demonstrated the technique by observing the sodium, Na, atom in a laminar premixed methane-air flame seeded with a sodium chloride, NaCl, solution.
REFERENCES


74. Hayhurst, A.N. and Kittelson, d.B. 1977), Combust. Flame, 28, 301


103. MacLachy, C.S. (1979), Combust. Flame, 36, 171


Note: The references listed here include some papers related to traditional measuring techniques that are not cited in the lectures of this course. They are cited in the entitled manuscript “Advanced measuring Techniques in Flames” Mohy S. Mansour.
PARTICLE IMAGE VELOCIMETRY MEASUREMENTS
OF PREMIXED METHANE-AIR FLAMES

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ABSTRACT

Particle Image Velocimetry (PIV) is a technique for measuring instantaneous velocity over an area (global measurement) in comparison to point velocity measurement over time using Laser Doppler Velocimetry (LDV). PIV provides information on flow visualization and associated structures such as velocity map/distribution, streamlines and vorticity. In this study, PIV was used for the first time to study an axially forced turbulent premixed methane-air jet flame. The PIV measurements were taken with a 532 nm narrow-band filter to reduce the radiation from the flame. The experimental methods and results of the study are presented and discussed.

1.0 INTRODUCTION

An understanding of the premixed turbulent combustion of natural gas or methane is essential since: (1) the characteristic dimensions and flow rates of most industrial equipment are often large enough for flows to be turbulent, and (2) many industries are now pursuing lighter hydrocarbon alternative fuels and the use of premixed combustion processes to reduce pollutant emissions [1]. In spite of the many prior studies on methane-air combustion [2-5], the fundamental mechanisms and kinetics involved in the premixed combustion process are not well understood. Despite extensive research work on turbulent flow structures, the interactions between the chemical reactions and the turbulent flow are not clearly understood. The current prediction models are not reliable, and much of the analytical work fail to properly handle the coupled non-linear fluid dynamic and chemical complexities. There is clearly a need for better understanding and more accurate and powerful approaches for addressing this very basic combustion problem. The ability to measure and predict the complex transport phenomena through detailed experiments and modeling is critical and needed. This study was undertaken using particle image velocimetry (PIV) to provide flow visualization and associated structures for a better understanding of the combustion process. The gas emissions from the combustor were also characterized to provide information on the chemistry of the process.

2.0 EXPERIMENTAL

2.1 Experimental Set-up

The schematic diagram of the experimental set-up is shown in Figure 1, and consisted of a gas feed and seeding system, a premixed combustor, an exhaust gas analysis system, and a particle image velocimeter (PIV). The premixed combustor consisted of two chambers. One was a stainless steel mixing chamber with a ceramic honeycomb flow straightener. The other was a water-cooled stainless steel combustor equipped with four quartz windows for flow visualization and PIV measurements. The two chambers were connected by a tunnel with the dimensions of
about 4 (1/4 (4 inches (length (width (height))(Figure 2). The width of the tunnel was adjustable up to the maximum value of 1/4". The tunnel acted as an additional mixer as well as the combustor nozzle. In this study, several different nozzle materials and sizes (widths) were tested. The flame/flow image was recorded by a cross correlation camera through the quartz windows. The camera was controlled by a computer through a PIV image processor interface (Figure 3).

Gas Feed System. The gas feed system consisted of gas sources (cylinders) and flow control systems. Commercial grade methane (>93% CH₄) produced by C&C Oxygen Co. (Chattanooga, TN) was used. The gaseous flow rates and the methane-air ratio were precisely controlled by an MKS gas control system (1179 A Mass-Flo Control, MKS Instruments Inc.), which consisted of a 50-slm (methane) and a 200-slm (air) mass flow controller, and a 647B multi gas controller.

PIV Measurement. The given flow rates of methane and air were injected into the mixing chamber from gas cylinders. To make PIV measurements, the flow field has to be seeded. About one third of the air was passed through the seeder, which was located upstream of the mixing chamber. The pre-dried titanium dioxide particles (with mean particle size of 0.3 (m) in the seeder was stirred by a small motor and carried by the air to the mixing chamber. The methane, air and titanium dioxide particles were thoroughly mixed in the mixing chamber with an average residence time of about 0.6 min and injected into the combustor through the ceramic honeycomb flow straightener and the tunnel nozzle. With or without the flame on, a pair of 532 nm YAG lasers were 'fired' with a pulse of 16 ns and the interval of 300 (s between the two laser pulses. At each laser pulse, the CCD camera was shot once and the image was stored in the computer. For the flame-on measurements, after considerable difficulties with the PIV measurements due to the strong background light of the flame which prevented identification and recording of the image of the seed particles, a 532 nm narrow-band width filter was mounted on the camera to block all of the light from the flame except that at 532 nm so that laser light scattered by the seed particles could be recorded and processed.

Two different camera lenses, a 50 mm, 1:1.4 and a 60 mm, 1:2.8, were used. Both gave good images. Since the 50 mm lens is more light sensitive, it was chosen for the measurements. In order to obtain high resolution images, the camera was placed at a point about 0.6 m from the center of the flame. At this point, the field of view covered only part of the combustor so three images were taken from three different positions for each test in order to measure the whole field of interest.

2.2 Experimental Procedures
The PIV measurements were carried out as follows: 1) The power source of the laser was turned on and the laser sheet focus was adjusted by using a black film paper. 2) The PIV system was calibrated with a stainless steel ruler, which was placed in the combustor at the laser sheet plane to provide a scale for the velocity vector. 3) The seeder was turned on by passing about 1/3 of the total air through it to entrain the titanium dioxide particles into the combustor, and 4) the PIV measurements were taken by firing pairs of 532 nm YAG lasers at specified time intervals and recording the images observed. In order to obtain reliable results, about 50 pairs of images were taken for each experimental condition. The same procedure was followed in the PIV
measurements for both the cold flow and hot flow (with flame) except that only air (without fuel) was fed into the combustor when the cold flow measurements were taken.

For each experiment at a specified set of conditions, in addition to the PIV measurements, the emissions from the combustor were characterized using Horiba gas analyzers for unburned hydrocarbons, NOx, O2, CO and CO2.

3.6 RESULTS AND DISCUSSION
3.1 Measurements without Flame

The image picture, velocity vector map and the deduced streamlines of a 40-slm cold air flow (without flame) showed that the premixed gas was injected from the nozzle to the combustion chamber and symmetrically flowed up, see Figures 4, 5 and 6. The 1.4 m/s jet of 4 mm width penetrated about 28 mm (7 D, where D is the width of the nozzle) above the nozzle without much disturbance. Figure 5 also illustrates that two large vortices were generated in the corner region where recirculation took place. In the region of 30 to 65 mm (7.5 to 16 D) above the nozzle, the vortices were formed on both sides of the main flow stream. The gases near the main stream moved up and the gases near the combustor wall moved down. The shedding of these vortices are believed to be responsible for the oscillation of the flame observed in the experiments.

As indicated in Figures 5 and 6, at the moment when the image was taken, it is believed that the main flow stream swung to the left side. As shown in the figures, on the right hand side of the jet, there existed a stronger vortex at a relatively lower position than that of the left-hand-side vortex. This stronger vortex produced the greater negative pressure in its center, which caused the main stream to swing to the right side at the next moment. It was also shown that the velocity of the jet was slowed down significantly, and the main stream became broader due to the entrainment of gases from the surrounding.

The vorticity map in Figure 7 indicates two strong vortices next to the main jet stream. The green color strip between the red and blue color regions in Figure 7 clearly indicate the original jet stream, which had almost the same width as the nozzle, 4 mm. On each side of the main stream, there was a 3 mm mixing region, where the stationary gas mixed with the main stream. This mixing region made the jet wider, as shown in Figure 6. When the gases were entrained into the jet from the surrounding, a negative pressure (vacuum) was produced, so the gases nearby moved in. This gas movement caused the main recirculation in the combustor, as shown in Figures 4, 5 and 6.

There are probably several different mechanisms by which the shed vortices influence or are directly responsible for the formation of stream turbulence. Some of the possible mechanisms can be discussed with the aid of Figures 4 and 5. It is assumed that the near-wake region consists of large stationary vortices or recirculation zones analogous to those given by the time average description illustrated in Figures 4 and 5. The shed vortices represent a dynamic flow superimposed on the outer stationary vortex established by the jet. Figure 5 was drawn to highlight the rotational motion of the shed vortices and it can also be viewed as a representation of the near-wake flow field at one instance in time.
3.2 Measurements With Flame

The radiation from the flame made PIV measurements difficult. Addition of the titanium dioxide particles made it even worse. Figure 8 shows that with the addition of the titanium dioxide particles, the flame of the premixed methane-air combustion was very bright. This broad band radiation was so strong that the PIV image could not be obtained in the traditional way. Therefore, all of the PIV measurements with flame were taken with a 522 nm narrow-band width filter.

Figure 9 shows that with the flame the jet quickly expanded and the flow speed significantly increased (see Figure 10). The average velocity of the fuel decayed as it moved downstream and entrained hot gases [6]. The combustible mixture began to break up into clouds or packets as it transitioned to turbulent flow. As the mixture packets approached the end of the recirculation zone and absorbed sufficient heat to ignite and burn as a packet of flame, the temperature rose rapidly. According to Equation 1, under stoichiometric conditions

\[
\text{CH}_4 + 2 (\text{O}_2 + 3.76 \text{ N}_2) = \text{CO}_2 + 2 \text{H}_2\text{O} + 7.52 \text{ N}_2
\] (1)

the moles of the exhaust gases from air-methane combustion are equal to the moles of the premixed gases. The gaseous pressure before and after the combustion should therefore be the same, which equals the ambient pressure. Thus, assuming ideal gas behavior, after combustion (T = 2000 K), the volume of the gases should increase to about 2000/298 = 6.7 times. As a result, the jet expanded and the mean velocity increased. Both factors led to a large flame structure.

The recirculation of the cold flow was caused only by molecular friction. In the combustion case, however, the gas near the flame was heated more and became lighter. These lighter gases moved up due to buoyancy, which accelerated the recirculation and made the recirculation more complicated, as shown in Figure 11. In addition to buoyancy effects which add order to the flow, the flame raises the gas viscosity by an order of magnitude resulting in the elimination of some of the turbulent structures. The mechanism of the formation of the vortices and turbulence with the flame system appeared different from that of the cold (without flame) flow. With the flame, some of the flame packets were entrained into the reverse flowing stream of the large stationary vortex and were transported upstream. As they moved upstream, the flame packets went through a period of acceleration and then began to decelerate as they approached the combustor dump plane. There was only one flow direction available for the flame packets to exit the recirculation zone established by the stationary vortex. The flame packets, or the products of combustion, were entrained by the mixture jet thus providing a source of heat and possible ignition of new fuel packets.

The centers of the stationary vortices were considered important because they directed the flow of the flame packets into the combustible mixture jet. Just before an active period of vortex shedding, the rotational velocity about the stationary vortex center increased. This seemed to be due to an increase in heat flux, hence pressure, in the recirculation zone by continued entrainment of the flame packets back into the recirculation zone as they attempted to escape. This
recirculation of the flame packets and the heat build-up continued until a vortex, containing flame packets, was shed downstream.

The difference in velocities of the flame packets and the jet gave rise to the formation of moving vortex that appeared to be shed from the dump plane. This shed vortex, as shown in Figure 12 looked like those observed in the shear layer experiments of Brown and Roshko [7]. As the shed vortex rotated, it picked up the flame packets as they are distributed around the combustor, thus making the shed vortex visible in the image picture. As one vortex was shed, another vortex was being formed. The vortex continued its motion downstream, decelerating as it approached the end of the recirculation zone.

3.3 Effect of Total Flow Rate on the Flame Structure

Six different total flow rates from 17 to 44 slm were tested at equivalence ratio \( \phi = 1 \). Since this is the first time a PIV technique is being successfully used for combustion flame measurements, much needs to be done to understand and interpret the results. So far, high spatial resolution quantitative measurements still cannot be obtained without the sacrifice of the size of the field of view. As the total flow rate increased, Figure 13 shows that the average velocity in the combustor increased. In addition, the gas temperature in the combustor also increased due to significantly higher heat input by the combustion process. The increases of both flow velocity and gas temperature enhanced the recirculation in the combustion chamber. Figure 14 shows that as the total flow rate increased, the jet stream expanded earlier, particularly near the nozzle, where the recirculation was the strongest. Finally, the streamlines obtained from a higher position in the flame (Figure 14) indicate that turbulence was significantly increased.

3.4 Emission Results

Figure 15 shows that the NOx concentration was heavily affected by the equivalence ratio \( \phi \). and had a maximum value, 58.8 ppm, at \( \phi \approx 1 \) and 27 slm of airflow. This is because the formation rate of NOx is mainly controlled by kinetic factors [8, 9], and the concentration of NOx in exhaust gases is mainly a function of combustion temperature. Under \( \phi = 1 \), the flame was measured to reach its highest temperature [10, 12]. As \( \phi \) moved from stoichiometric ratio to either fuel-lean or fuel-rich, the flame temperature decreased. This resulted in a maximum in the NOx concentration curve similar to that of CO2. It should be noted that thermal NOx reached its maximum value at a lower \( \phi \) than that of CO2. This divergence was also found in the literature [8] and in the previous studies in our lab [10, 12]. As the total flow increased, the total energy released from the combustion increased and the combustion temperature increased. As a result, in the fuel-lean region, the NOx concentration in the exhaust increased with flow rate. However, in the fuel-rich region, the increase of the total flow made incomplete combustion worse, which led to lower combustion temperatures and, hence, NOx. The combined effects resulted in the fuel-lean-side shift of the NOx concentration curve as the total flow increased, as shown in Figure 15. The unburned hydrocarbon, O3, CO and CO2 in the emission exhaust of premixed methane-air combustion under different conditions were also investigated. The detail information can be found in Yeboah et al [12].
4.6 CONCLUSION

- The flow velocity distributions, streamlines and vorticities were successfully measured and recorded using a Dantec Dual Cavity Particle Image Velocimeter (PIV). By using a 532 nm narrow-band width filter, where 532 nm is the laser wavelength used for the PIV measurement, most of the bright radiation from the flame were filtered out, which greatly reduced the background light noise from the flame making it possible to determine and record the titanium dioxide scattering light from the laser.

- 40 slm cold air flow at 1.4 m/s jet penetrated 28 mm (7 D, where D is the width of the nozzle) above the nozzle without much disturbance. In the region of 30 to 65 mm (7.5 to 16 D) above the nozzle, vorticities were formed on both sides of the main flow stream. On each side of the main stream, there was a 3 mm mixing region, where the stationary gases mixed with the main stream gas, which made the streamlines of the flow appear about twice as wide as the nozzle.

- With the flame, the flow jet quickly expanded several times in volume, and the flow speed significantly increased from its corresponding cold flow value. Some of the flame packets were entrained into the reverse flowing stream of the large stationary vortex and were transported upstream. Just before an active period of vortex shedding, the rotational velocity about the stationary vortex center increased. As the shed vortex rotated, it picked up the flame packets around the combustor, thus making the shed vortex visible in the image picture. As the total inlet gas flow rate increased from 17 to 44 slm (0.59 to 1.5 m/s), the average velocity and temperature inside the flame increased, which enhanced the recirculation and turbulence.

- The NOx formation was mainly dependent on the combustion temperature, and reached its maximum, 58.5 ppm, at the equivalence ratio (φ = 1) and air flow of 27 slm. The NOx concentration decreased significantly as the operation moved away from stoichiometric conditions. As the total flow increased, the NOx curve shifted to the fuel-lean region.
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REFERENCE


Fig. 1 Schematic of the experimental setup

Fig. 2a Pictures of the methane-air premixed combustor (Side and Top views).
Fig. 2b  Pictures of the methane-air mixing chamber (Side and Top views).

Fig. 3  Photographs of the Dantec flow map particle image velocimeter (PIV).
Fig. 4 The image picture of the cold flow (without flame) (total air flow = 40 slm, 122 x 4 mm marble nozzle.)

Fig. 5 The PIV velocity vector map of the cold flow (without flame) (total air flow = 40 slm, 122 x 4 mm marble nozzle.)
Fig. 6  The PIV streamlines of the cold flow (without flame) (total air flow = 40 slm, 122 x 4 mm marble nozzle).

Fig. 7  The PIV vorticities of the cold flow (without flame) (total air flow = 40 slm, 122 x 4 mm marble nozzle).
Fig. 8 The picture of the premixed methane-air combustion flame ($\Phi = 1$, total premixed-gas flow = 40 slm, 122 x 4 mm marble nozzle.)

Fig. 9 The PIV streamlines of the hot flow (with flame) ($\Phi = 1$, total premixed-gas flow = 40 slm, 122x4 mm marble nozzle.)
Fig. 10  The PIV velocity vector map of the hot flow (with flame) ($\Phi = 1$, total premixed-gas flow = 40 slm, 122x4 mm marble nozzle.)

Fig. 11  The PIV verticals of the hot flow (with flame) ($\Phi = 1$, total premixed-gas flow = 40 slm, 122x4 mm marble nozzle.)
Fig. 12  The image picture of the hot flow (with flame) ($\Phi = 1$, total premixed-gas flow = 40 slm, 122 x 4 mm marble nozzle.)
Fig. 13  Effect of the total gas flow on the velocity of the combusted gases ($\Phi = 1.122 \times 4 \text{ mm marble nozzle}$.)
Fig. 14a  Effect of the total gas flow on the streamlines of the combusted gases (the lower part of the combustion field, $\Phi = 1,32 \times 4$ mm marble nozzle).
Fig. 14b  Effect of the total gas flow on the streamlines of the combusted gases (the upper part of the combustion field, $\Phi = 1.122\times4$ mm marble nozzle.)
Fig. 15  Effect of the total premixed-gas flow rates on the Nox concentration
CO2 – TEA LASER-BASED LIDAR DIAL SYSTEM
FOR THE DETECTION OF HYDROCARBON POLLUTION
IN THE ATMOSPHERE

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ABSTRACT

We present the technology and the configuration of the home build Lidar Dial system. Campaign results will also be presented for the case of Ethylene, Ammonia, and possibly Ozone. Long path integrated measurements of these pollutants against a topographic target will be discussed.
LASER DOPPLER VELOCIMETRY AND HIGH-SPEED VIDEO IMAGING SYSTEM FOR COMBUSTION AND EMISSION CONTROL RESEARCH

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ABSTRACT
Laser Doppler Velocimetry (LDV), which provides point measurements of velocity over time, and high-speed video imaging are two powerful diagnostics for flow visualization of combustion and emission control processes. LDV was used to study an axially forced turbulent premixed methane-air jet flame and the results of the LDV studies compared to those obtained with particle image velocimetry (PIV). In addition, the application of a high-speed video imaging system, Kodak Ektapro Motion Analyzer, to study droplet combustion behavior under supercritical conditions and non-thermal plasma discharge for NOx removal and control are presented and discussed.

1.0 INTRODUCTION
The need and ability to make accurate and detailed experimental measurements in practical combustion systems involving high-temperature, multi-species, multi-phase turbulent flows with chemical reactions present the combustion scientist with formidable challenges. In the past, probes in hostile environments, as well as the tendency of probes to modify the flows they are intended to measure, have limited their accuracy and complicated the interpretation of results. Laser diagnostics have opened new horizons for the combustion and fluid flow scientist. Through the use of lasers, it has become practical to make accurate measurements of temperatures, concentrations, densities, and velocities with high spatial and time resolutions in practical combustion and fluid flow situations, without disturbing the flow field under study. These innovative measurement technologies and instruments have undoubtedly improved the understanding of combustion processes, which will eventually lead to the development of more efficient and environmentally acceptable combustors.

Fluid flow research calls for the development of theoretical models that are capable of describing the complex flow phenomena such as those in the compressor, around an aircraft body, and reacting flows in the combustion chamber. On the other hand, the theoretical or numerical results generated by computational fluid dynamic (CFD) research need to be verified and the computer codes validated by experimental data. The development of appropriate measurement techniques that can provide the experimental data needed to guide the theoretical efforts becomes, again, critical for the success of research.

Clark Atlanta University has a well-developed Combustion and Emission Control Laboratory. Current research projects include studies on turbulent reacting flows, pulsed combustors, non-thermal plasma discharge, droplet combustion, and low-NOx combustor development. The two instruments described in this paper, a three-dimensional Laser Doppler Velocimeter (LDV) and a high-speed imaging system, have been used for most of these studies. The facilities have enhanced and expanded the scope of the research CAU can undertake and
empowered CAU to successfully undertake research in critical areas as fluid dynamics, combustion and propulsion, and chemical kinetics.

2.0 INSTRUMENTATION

2.1 Three Dimensional Laser Doppler Velocimeter

Laser Doppler Velocimetry (LDV) is a powerful technique used for highly accurate measurements of fluid velocity in liquid or gaseous flows. Scattered light from particles passing through the probe volume has a Doppler frequency proportional to the particle velocity. Very small probe volumes can provide highly resolved velocity profiles and allow measurements close to a wall or object in the flow. Measurements can also be conducted in extremely harsh environments such as in combustion processes and in explosions.

The three dimensional LDV system used in this study is a state-of-the-art fiber optic system designed and manufactured by TSI Inc., St. Paul, MN. The system provides superior alignment stability and is designed to virtually eliminate the need for internal adjustments. The optical transmitter is rugged and easy to set up. Frequency shifting applied to the input beams acts to offset the Doppler frequency, providing improved dynamic range and allowing distinction between forward and reverse flow directions. The 3-D system uses different wavelengths to form independent overlapping probes for orthogonal flow directions. This greatly reduces the time required for mapping multi-dimensional flows. In addition, fiber optic probes are used to isolate the transmitter and receiver optics from their electronics. This enables application in harsh environments which protect the more sensitive electronic and electro-optical system component.

The LDV signal processor, Doppler Signal Analyzer (DSA), provided by TSI employs the latest innovation in analog and digital electronics for maximum processing efficiency and reliability. Trans-impedance pre-amplifier, high speed Analog-to-Digital Converters (ADC), advanced array processors, and the Fourier Transform Burst Detector technology used in the design have contributed to the outstanding performance. The DSA is capable of processing Doppler frequencies as high as 150 MHz. Two 160 MHz ADC’s perform simultaneous sampling of the quadrature mixed signals, resulting in an equivalent sampling frequency of 320 MHz. The DSA has an operating bandwidth of up to 145 MHz. This is superior to processors which have operating bandwidth much smaller than their frequency range. The DSA implements the optimal method of frequency estimation, the Discrete Fourier Transformation, to determine the Doppler frequency, and then the velocity. The Fourier transform involves the matching of noisy Doppler signal with sine waves of discrete frequencies.

This is a distinct advantage over other signal processing methods because the effect of the noise can be downplayed by correlating the signals with pure signals instead of noisy signals. Consequently, accuracy is maintained, even in difficult environments where the signal to noise ratio (SNR) may deteriorate to below -6 dB. In addition, reliable measurements can be obtained independent of the number of signal cycles recorded, and the DSA does not produce a frequency bias when the SNR deteriorates. The DSA incorporates an innovative signal burst detection system that uses both the Fourier transform and signal power in the time domain. The Fourier
Transform Burst Detector performs up to 20 million Fourier transforms per second. It eliminates
the dependence of the signal detection on the signal and noise amplitude, favoring the SNR.

2.2 High Speed Imaging System

The high speed imaging system acquired is a Kodak EktaPro Motion Analyzer which
consists of three primary components: an imager, a processor, and a monitor (Eastman Kodak
Company, NY). The system is a powerful imaging tool designed to capture events at 1,000 to
12,000 pictures per second with resolution of 192 x 239 pixels, in bright sunlight to near darkness
(1.5 lux). The analyzer allows simultaneous recording of two views of the same subject, or two
separate but related subjects, by simply adding another imager. It has a multi-channel data link
port, allowing the measurement of voltage levels of actuators, sensors and other
electrical/electronic devices with dynamic characteristics, and recording of data along with the
video images.

The high speed imager features extremely fast electronic shutter speeds, with exposures
as short as 10 microseconds to “freeze” an object in motion. The motion analysis processor
EktaPro EM can capture and store 1,000 full-frame or 12,000 split-frames per second. The stored
images can be played back at a rate ranging from single step up to full speed in both forward and
reverse mode, be displayed on a standard video monitor, copied to a VCR for archiving, outputted
to video printer or downloaded to a computer workstation for display and digital image analysis.
The Kodak EktaPro motion analysis workstation provides powerful software for digital image
enhancement and quantitative motion analysis.

3.0 RESEARCH SUPPORTED BY THE ACQUIRED INSTRUMENTATION

Several research projects, such as turbulent premixed combustion, non-thermal plasma
discharge, and droplet behavior under supercritical conditions, have been carried out with the laser
Doppler velocimetry and high speed imaging system. Some of the research results from these
projects are discussed below.

3.1 Turbulent Premixed Methane-Air Combustion

An understanding of the premixed turbulent combustion of natural gas or methane is
essential since: (1) the characteristic dimensions and flow rates of most industrial equipment are
often large enough for flows to be turbulent, and (2) many industries are now pursuing lighter
hydrocarbon alternative fuels and the use of premixed combustion processes to reduce pollutant
emissions [1]. In spite of the many prior studies on methane-air combustion [2-8], the fundamental
mechanisms and kinetics involved in the premixed combustion process are not well understood.
Despite extensive research work on turbulent flow structures, the interactions between the
dissipative reactions and the turbulent flow are not clearly understood. The current prediction
models are not reliable, and much of the analytical work fail to properly handle the coupled non-
linear fluid dynamic and chemical complexities. There is clearly a need for better understanding
and more accurate and powerful approaches for addressing this very basic combustion problem.
The ability to measure and predict the coupled effects of
complex transport phenomena through detailed experiments and modeling is critical and needed.
Particle image velocimetry (PIV) and Laser Doppler velocimetry (LDV) are two of most advanced techniques of unveiling flow and associated structures. PIV measures velocity over many points - a cross section - at one instant in time and offers a global image, while LDV provides the detailed time history at a point and gives a point information at each time. Although PIV and LDV work by different principles, they complement each other well in many application areas. With the PIV measuring technique, the velocity of a flowing medium is measured by recording the displacement of small particles carried with the flow and subsequently analyzing the particle displacements recorded. Particles embedded in a region of the flow are illuminated by two or more short laser pulses fired with a known time separation. The particle positions are recorded by means of a CCD camera. The particle displacements in the flow field are found from the displacements in the image plan. Knowing the magnification of the imaging and the time separation between the laser pulses, the velocity projections on the measuring plane are found.

The schematic diagram of the experimental set-up for the turbulent premixed methane-air combustion using the LDV measurement systems is shown in Fig. 1. The LDV system used in this study was a TSI three-component (3-dimensional) Laser Doppler velocimeter (Thermal Systems Inc., St. Paul, MN), consisting of the compact TRCF-3 ColorBurst multicolor beam separator, the ColorLink multicolor receiver, the S75-3 IFA 750 processor, the PermaFiber fiberoptic probes, and the FIND and PHASE data analyzer. The system measured the three components (dimensions) of the instantaneous velocity. The strong beams of a multicolor argon-ion laser (green/514.5 nm, blue/488 nm and violet/476.6 nm) were used to measure the velocity components. The laser beams were provided by a 5 W Coherent Innova-90 argon-ion laser (Coherent Inc., Santa Clara, CA), and split by a TSI TRCF-3 ColorBurst. The three-component velocities were measured by a dual-axis fiberoptic system, consisting of a 83-mm diameter two-component fiberoptic probe for 514.5 nm (green) and 488 nm (blue), and a 83-mm diameter single-component fiberoptic probe for 476.5 nm (violet). Both probes had the following parameter values: beam spacing - 5 mm; focal length - 350.0 mm; half angle - 4.096 degree; receiver focal length - 310.0 mm; and receiver optic axis elevation - 1.0 mm. The laser beam diameter at the front of the probe optics was 2.2 mm. The fringe spacing for channels 1, 2, and 3 (green, blue and violet) were 3.062, 3.416 and 3.332 μm, respectively. The two probes were mounted on a three-axis traverse at a certain angle. For each dimension measurement, two same-wavelength laser beams at a certain angle were shot simultaneously. When the two laser beams hit a moving particle, it produced a Doppler shift, which was reflected back to the optic probe for velocity calculation.
As the LDV measurement is not affected by background lights, there was no need for a light filter as was required for the PIV. Because the LDV is a point measuring technique, a traverse was used to move one or two fiber optic probes in three orthogonal directions. The traverse provided maximum 600-mm travel distance with 0.01-mm resolution on each direction. The two probes could be adjusted for a wider range of focal distances. Because of the symmetry in the X direction, only two dimension measurements (Y and Z directions) were needed in this study. One probe with the 514.5 nm (green) and 488 nm (blue) lasers was used for the Z and Y directions, respectively. The probe used for the Y and Z measurements was oriented in the X direction.

Since LDV is a point measuring method, several hundreds of measurements were taken and used to make a flow structure plot by means of the computer software “TecPlot 7.5” (Amtec Engineering Inc, Bellevue, WA), as shown in Fig. 2. Figure 2 indicates that the main stream of the cold flow from the LDV measurements was about 4 mm wide, close to the nozzle width, and moved up to about 65 mm (16 D) above the nozzle without much disturbance, which is similar to the results from the PIV measurements. Beyond the 65 mm, the main stream became narrower and no large flow vortices were recorded, which was different from the PIV measurements. For the PIV measurements, in the region of 65 mm above the nozzle, the main stream became wider due to the vortices formation on each side [6, 9]. It is believed this may be due to the low LDV sensitivity to slow flows. According to DeCroix and Gould [10], <0.5 m/s flow velocities are problematic for LDV measurements. In addition, the seed particle concentration and size of the
LDV seeding system were not controlled as well as PIV system due to its longer measuring time, which may also have contributed to the lower LDV sensitivity.

![LDV velocity vector map](image)

**Fig. 2** The LDV velocity vector map of the cold flow (without flame) (linear airflow = 1.4 m/s, 122 × 4 mm marble nozzle).

The contour map of the cold flow for the LDV measurements is plotted in Fig. 3, and shows similar results to the vector map described above. The studies with flames are currently in progress.

### 3.2 Optimization of Nonthermal Plasma Discharge Electrochemical System

Nonthermal plasma discharge (NTPD) is one of the promising innovative technologies to destroy hazardous air pollutants and criteria pollutants contained in gas streams prior to atmospheric dispersion. When released into the atmosphere, the group of compounds collectively known as nitrogen oxides or NO\textsubscript{x} contributes to photochemical smog, acid rain and ground-level ozone. Combustion processes are a primary source of NO\textsubscript{x} emissions and finding a cost-effective technology to remove NO\textsubscript{x} from combustion exhaust streams is essential. Within the Air Force infrastructure, diesel-powered aerospace ground equipment (AGE) have been identified as significant sources of NO\textsubscript{x}. Given the operational constraints of AGE, an Air Force study identified the Non-Thermal Plasma Discharge or NTPD as a promising technology for NO\textsubscript{x} removal. As part of a program to optimize an NTPD system for this particular application, an
investigation of the affect of discharge gap spacing on the electrical and chemical processes that occur in NTPDs was initiated. A number of experiments were performed to examine how the gap spacing affects the NO\textsubscript{x} removal efficiency, discharge characteristics, and chemical reactions in a NTPD device. The schematic of the double dielectric barrier discharge reactor is shown in Figure 4. The gap spacings ranging from 0.8 to 4.0 mm were considered in this study. An optimum gap spacing for NO\textsubscript{x} removal was observed at approximately 2 mm and based on the experimental data a physical explanation for the optimum was developed.

![Figure 3](image)

**Fig. 3** The LDV velocity contour map of the cold flow (without flame) (linear airflow = 1.4 m/s, 122 x 4 mm marble nozzle).

![Figure 4](image)

**Fig. 4. Schematic of DDBD Reactor**

A schematic of the overall experimental setup is given in Figure 5 [11, 12]. A KODAK EKTAPRO High Speed Intensified Imager System and Nikon Micro lens were used to study the microdischarges. Specifications for the camera system include a frame rate of 30-6000 fps, a spectral sensitivity of at least 50% peak from 440 nm to 700 nm, and a variable gate time from 10-
5000 μsec. Output from the imaging system was recorded on videotape via a 1/2" VHS VCR. The system was used to view the microdischarges from points both perpendicular and parallel to the breakdown channel.

![Schematic of NTPD experimental setup.](image)

Photographs, which were taken with the intensified high-speed imager in framing mode, revealed details of the microdischarge behavior [13]. The spectral range of the imager was from 400 to 800 nm and we assumed that the microdischarge images in this range represent the primary electron stream forming the discharge channel. It is important to note that the duration of the discharge image reflects only the integration of the excimers life within the channel and not the duration of actual charge transfer through the channel. During a single half power cycle both the number and the physical dimensions of the microdischarges could be obtained directly by the imager. In order to extract further information from the optical observations the characteristics of the microdischarges were related to the transferred charge. For this analysis the double dielectric barrier discharge (DDBD) electrode configuration was presumed to be symmetric and we further assumed that all of the available surface charge was transferred through microdischarges in which chemical reactions were initialized. The specific reactions taking place within the microdischarges are determined by electron-molecular/atom collisions.

A series of microdischarge images at different gap widths are presented in Fig. 6 [13, 14]. When obtaining these images, the residence time of the gas in the DDBD device was fixed at
0.46 s. The fixed residence time was accomplished by changing the inlet flow rate when changing
the gap spacing. The input power, driving frequency, and flow temperature were also fixed in
each case, as was the gas mixture. The specific conditions under which the images in Figure 6
were obtained are given in the figure caption. Notice that with increasing gap spacing the radius,
r, of the discharge increased significantly, while the number of discharges per half cycle
dramatically decreased. The radius was found to vary from approximately 90 µm at the 1 mm gap
width to 340 µm at the 4 mm gap width. The frame rate for these images was 1000 fps and the
gate time was varied from 20 to 200 µs to obtain the clearest image.

![Image of microdischarges at different gaps](image)

**Fig. 6** High-Speed Images of Microdischarges at Different Gap
Widths: Gas composition: 1000 ppm NO, 2000 ppm H₂O, 10%
O₂, N₂ balance, Room Temp, 1 atm, Power = 5 Watts,
Frequency = 400 Hz, Residence time = 0.46 s

3.3 Study of Droplet Behavior under Supercritical Conditions

Droplet and spray combustion dynamics play critical roles in the operation of liquid
rockets, advanced gas turbines, and diesel engines. Because of their direct relation to practical
spray combustion devices, the behaviors of liquid droplets in environments at supercritical
pressure and temperatures under normal and microgravity conditions have long been of important
research interest. About three decades have passed since the first experimental investigation of free
droplet combustion under microgravity was presented by Kumagai and his co-workers [15]. Since
then, extensive research has been conducted [16-23]. However, since there are still many
difficulties involved in conducting droplet combustion experiments, many questions still remain
unanswered. One of the experimental difficulties is the ignition of a free droplet without
disturbing its shape and movement. Kumagai et al [24] used an electrical spark to ignite a
suspended droplet at ambient pressure; even so the electric spark still had some effect on the
droplet's shape. The most recent and detailed work was conducted by Litchford and his co-
workers [25]. Litchford et al used a pre-heated gas jet which came from the bottom of the
combustor to ignite the suspended droplet through convective heating. During the ignition
process, the droplet was deformed by the aerodynamic force of the hot flow.

The droplet formation and release under high pressure and/or high temperature are also a
difficult problem for droplet study. Litchford et al [25] and Kumagai et al [26] used a tiny tube to
transfer the liquid fuel to a metal/quartz wire frame which was used for the droplet suspension.
Because of the surface tension between the tube and the liquid, the droplet was difficult to transfer to the suspension wire, and the transferred droplet size was difficult to control. Further, after the droplet was transferred to the suspension wire, it was more difficult to release to a free droplet [24].

A novel and versatile droplet experimental setup was developed at Clark Atlanta University [27], which consists of a liquid pressurizing and transfer system, a high pressure/temperature chamber, a droplet formation, release and ignition system, and a high-speed imaging system. The setup provides quiescent or convective environments under supercritical pressure and temperature conditions. Quiescent environment droplet gasification tests and convective environment droplet combustion tests were conducted under sub- and supercritical pressures with the setup. Specifically, the gasification rates of 1.5-mm-diameter suspended droplets were measured under different conditions (e.g., sub and super critical pressures). The characteristics of a free-drop non-combusting droplet (~1.5 mm diameter) and a free-drop combusting droplet were studied using a high-speed image system [27]. The images of droplet gasification and combustion revealed interesting phenomena and provided better understanding of the droplet behavior in sub and supercritical pressure environments. The preliminary results show that pressure has a significant effect on the characteristics of droplet gasification and combustion, such as the oscillatory deformation of a free-drop droplet, the buoyancy effects and flame propagation of a combusting free-drop droplet.

The experimental set-up is shown in Fig. 7, which consists of a liquid-fuel supply system, a gas pressure-control system, a droplet formation system, a high-pressure chamber, an electrical igniter, and a high-speed CCD video system. Hexane was used for this preliminary study, which has a critical temperature of 507.7 °C, and a critical pressure of 436.6 psi (3.01 MPa) [28]. The experiments were carried out at pressures from 14.7 to 1200 psi, which covered sub and supercritical pressures of hexane.

The volumes/diameters of a suspended droplet were measured under different experimental conditions of 1000 frame/second and different pressures to measure its evaporation (gasification) rate. Figure 8 shows that the square of the diameter of the droplet vs time is a straight line in most parts of the gasification period, because the gasification rate is proportional to the surface area of a droplet. However, Fig. 8 indicates that after their diameter square reduced to about 0.50 mm² (~0.8 mm in diameter) at 200 and 800 psi pressure, the gasification rate increased by a factor of about three because of surface tension increase. Figure 8 further shows that the gasification rate at 500 psi pressure was more than double those at 200 and 800 psi. This is thought to be the effect of supercritical conditions.
Fig. 7  Schematic of the experimental setup of droplet behaviors under supercritical conditions

Fig. 8  The changes of the surface areas (diameter square) of droplets with gasification time under different pressures.
When a droplet was released from the thermocouple, it started to fall. The whole process was recorded by the high-speed video system at the recording speed of 1000 frame (picture) per second with an exposure time of 30 microseconds. By replaying the recorded image at a much slower speed (e.g., 1 – 30 frame/sec), the shape and speed of the falling droplet were measured. It was found that during falling, the shape of a falling droplet was oscillating in the vertical direction. The magnitude of the oscillation changed with the system pressure, which reached its minimum at the droplet’s supercritical pressure. From the recorded video images, it was observed that the system pressure has significant effects on the combustion of a free falling droplet. As the system pressure increases, the falling speed of a droplet proportionally decreased. When the chamber pressure was increased to a certain value (~200 psi), after falling below the ignitor ring for a distance, the burning droplet floated up. As the chamber pressure further increased, the distance that the burning droplet would fall below the ignitor ring decreased. As a combination effect, at a fixed time after its ignition, the distance of a free-burning-droplet falling-down decreased, as shown in Fig. 9. As the chamber pressure approached the droplet’s supercritical pressure, the free burning droplet virtually stayed at its ignited position (Fig. 9).

Fig. 9 The effect of the system pressure on the falling orbit of a free-falling burning droplet.
4.0 CONCLUSIONS

- A laser Doppler velocimetry system and a high speed imaging system have provided an integrated diagnostic system for flow visualization in the areas of combustion, propulsion, emission control, chemical kinetics and fluid dynamics.

- LDV is a point measuring technique and uses the Doppler principle. The flame's strong background light had little effect on its measurements. LDV is not as sensitive as PIV for the relatively slow flow, but it can provide three-dimensional velocities of a flow and the velocity history of a point, while PIV can provide only two-dimensional velocities. Similar to PIV, LDV has to use particle seeds for its measurements. The conditions of particle seeds are essential for both PIV and LDV measurements, but it is more critical for LDV measurements due to its longer measuring time. While PIV used either TiO$_2$ or Al$_2$O$_3$ as the seeds, Al$_2$O$_3$ particles were preferred for LDV measurements because they did not aggregate in the air. A narrow size range in a few micrometers or sub-micrometers should be used for LDV measurements.

- For the 40 s/$^-$m cold airflow at 1.4 m/s, the jet stream measured from LDV had 4 mm of width (1 D). The jet became narrow at 60 mm (12 D) above the nozzle, which was considered the formation of large vortices. No vortex stream was recorded in the LDV result, while the PIV measurements gave the two vortices on each side of the main stream. The difference was probably caused by the LDV low sensitivity in the slow flow.

- Non-thermal plasma discharges are increasingly being utilized for the processing of hazardous gas streams. This study indicated that gap width can be considered one of the major factors affecting the physical properties and performance of dielectric barrier discharges. In order to evaluate the effect of gap width on NO removal in combustion gas streams, both the physical properties of microdischarges and the NO removal efficiency were investigated at gap widths ranging from 0.8 to 4.0 mm. Photographic studies showed that the radii of the microdischarge footprint and cylindrical channel both increased linearly with gap width while the number of discharges decreased with increasing gap width.

- High speed images of droplet gasification and combustion revealed many interesting phenomena and provided better understanding of the droplet behavior in sub and supercritical pressure environments. The gasification process of a suspended droplet was studied under different conditions. A free falling droplet was ignited without disturbing its shape and movement. The combustion process of a free droplet including ignition under different conditions, such as pressure and temperature were analyzed.
ACKNOWLEDGEMENT

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CASE STUDY
COMBUSTION PROCESSES AT
TEMA OIL REFINERY (TOR) LTD

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ABSTRACT

The presentation focuses on current combustion technology and practices at Tema Oil Refinery (TOR) Ltd. As well as the on-going effort to improve efficiency with a view to reducing environment emissions. TOR’s combustion systems-boilers, furnaces, and associated auxiliary equipment are described. Combustion fuels and burner management systems and the control of these to ensure efficiency are presented. Monitoring and measuring techniques to ensure compliance with environmental requirements as well as TOR’s safety requirements vis-à-vis international Codes and Practices are also discussed.

1.0 INTRODUCTION

1.1 MISSION STATEMENT

The mission of Tema Oil Refinery (TOR) Ltd. is to refine crude oil into petroleum products and store them for distribution in the domestic market in a safe, efficient and cost-effective manner by applying process which are environmentally friendly.

In furtherance of this, TOR is expected to be one of the most efficient refineries in the West Africa Sub-region by:

(a) Making the best use of its available resource
(b) Maintaining a strict and cost-conscious maintenance culture
(c) Keeping abreast with modern refining technology to achieve maximum yield from crude inputs and ensuring that our products are of the right specifications.
(d) Ensuring manpower development and adequate compensation for all categories of employees in the organisation.
1.2 BRIEF OVERVIEW OF PROCESS AT TEMA OIL REFINERY

The Tema Oil Refinery was conceived in 1960 as part of the Ghana Government's Industrialization programme. Thus, the Government of Ghana, in conjunction with the Ente Nazionale Italiano per la Refinazione dei Carburanti (ENIRC) and the Italian company, SNAM, decided to form the Ghanaian Italian Company (GHAIP) with the object of carrying on refining in the country.

In December 1961, GHAIP entrusted a consortium of firms, consisting of SNAM progetti, SAIPEM and NUOVO PIGNONE, with the construction of a refinery at Tema capable of processing the most varied forms of crude. The capacity was 1,250,000 tons of crude oil per year. By the middle of 1963, the refinery had been completed and it covered a total area of 440,000 square meters.

1.3 THE PROCESS

The Tema Oil Refinery is linked to an oil jetty at the Tema Harbour by a 24 inches diameter crude oil pipeline. There are other products lines of 14, 10, and 6 inches diameter for export and import of finished product. When the ships arrive at the harbour inspection are done for quality and quantity. Then the fuel is pumped through pipelines into the floating roof storage tanks. As there is a sizeable amount of water in the crude, it is allowed to settle for two days before it is ready for processing.

1.4 REFINING

The crude is pumped from the storage tank to the TOPPING UNIT where it is gradually heated in a train of heat exchangers from ambient temperature to 330-350 degrees centigrade. It is then distilled at approximately atmospheric pressure into various fractions:

- LPG 2%
- VIRGIN NAPHTA 25%
- S. R. KEROSENE 14%
- GAS OIL 33%
- REDUCED CRUDE 26%

The Naphtha from the Topping Unit is further treated in the Reformer Unit where the Octane level is raised to meet the market specification. Refined products from the processing units are stored into various storage tanks where the products are prepared to market specifications.

1.5 FINISHED PRODUCTS

1. LIQUEFIED PETROLEUM GAS (LPG)- This is commonly called GAS and is made up of 20% propane and 80% by volume of butane gas. It is used as domestic, commercial and industrial fuel.

2. MOTOR GASOLINE (Petrol)- These meet the need of cars. Premium Gasoline (Super) caters for engines with high revolutions per minute.
3. **KEROSENE** - This is a refined petroleum distillate suitable for use as an illuminant where burned in a wick lamp.

4. **AVIATION TURBINE KEROSENE** - This is a grade of kerosene of such composition and characteristics that is suitable for use as aviation turbine fuel.

5. **INDUSTRIAL DIESEL OIL** - A blend of Gas oil and residual Fuel Oil (about) 70% of Gas Oil, and 30% by weight of fuel oil.

6. **GAS OIL (Diesel Oil)** - A petroleum distillate with a lower viscosity range between that of kerosene and residual fuel oil. It is suitable as fuel in high-speed Diesel engines.

7. **INLAND FUEL OIL** - This is burner Fuel Oil of lower viscosity than Residual Fuel Oil generally obtained by blending Residual Fuel Oil with petroleum middle distillates.

8. **INLAND FUEL OIL (Buicer C)** - This is a high viscosity oil obtained as a residue from the distillation of crude oil.

It is needed mostly for industrial heating, Furnace Boilers etc. and pre-heating to permit pumping and additional pre-heating to permit atomizing.

### 1.6 ELECTRICAL POWER GENERATOR AT TOR.

As part of the conceptual design of the Refinery a cogeneration facility consisting of two steam turbine generators each rated at 1.3 MW were installed to provide the power needs of the Refinery. After over 35 years of service these two turbine generators have become inefficient and have been breaking down so often. Thus with the conceived revamping of the refinery and the consequential increase in power demand a new 6.5 MW steam turbine generator was installed in 1996 to supply the refinery power needs. The capacity of this generator is at present in excess of the refinery demand and an agreement is being concluded with Electricity Company of Ghana to buy the excess power.

### 1.7 WHAT IS NEW

The Crude Distillation Unit (CDU) has been revamped from 28000 to 45000 Barrels per Stream Day (BPSD). With the objective of making the most out of the barrel of crude, TOR aims at going into Secondary Conversion Process. In the light of this, a contract has been signed with a consortium of firms namely SK Engineering and Samsung Corporation of South Korea for the building of RFCC (Residual Fluid Catalytic Cracking) Unit to convert the Residual Fuel Oil from the CDU into more valuable products: Gasoil, Gasoline and LPG. The Reforming Unit is also looking at increasing its capacity of the refinery to handle the increased Naphtha production from the Revamped CDU.
2.9 COMBUSTION SYSTEMS

Two main areas employ combustion systems in TOR’s operations. These are Boilers and Furnaces.

2.1 BOILERS

Water-tube boilers at the Power Plant /Utility section produce super heated steam primarily for refining processes and to drive turbine generators to produce electric power as a co-generation facility. Presently in operation are three boilers each with maximum capacity rating of 20 ton per hour of superheated steam. The steam output pressure is 40 bar and temperature of 400 °C.

2.1.1 TYPE OF BOILERS

The 3 boilers are D-type water-tube with left-handed furnace. They are designed for combined fuel gas and fuel oil firing. The constructional features of the boiler include:

1. Upper drum
   Lower drum
2. Steam tubes
3. Down comer tubes
4. Radiation superheated tubes
5. Convection superheating tubes

The furnace floor is covered with refractory laid on bottom tubes. The convection section is located alongside the combustion chamber. Fuel gas ducts which are refractory lined connect the fuel gas outlet on the convection section bottom to the air preheater and stack. The boiler manufacturers are Fontana, SPA of Italy. Presently under construction are 2 new boilers- a 35-ton per hour O-type boiler from INDECK POWER COMPANY of USA and a 60-ton per hour D-type from FOSTER WHEELER of Canada. Fig. 1 illustrates the constructional features of a typical D-type boiler in use at TOR.

2.1.2 BURNERS

Each boiler is equipped with 2 oil-fuel gas burners. The burners are the suspended flame type, remote operated register, gas pokers, one oil gun, steam atomised skewjet and permanent gas pilot ignitors. The burner manufacturer is AIR OIL FLARE GAS of U.K.

Fig. 2 & 3 show sectional view of the sprayer body assembly and skewjet atomiser assembly.

2.1.3 PREHEATERS

Vertical axis electric motor gear drive
FIG. 2. SECTIONAL VIEW OF 5000 SERIES SPRAYER BODY ASSEMBLY FOR SKEWJET ATOMISERS.
2.1.4 COMBUSTION CONTROL

The boilers are equipped with Forced draft fans with electric motor and steam turbine drives. Combustion airflow is automatically operated and controlled by inlet guide vanes, which are pneumatically actuated remotely. The air registers are normally fully opened.

2.2 FURNANCES

Combustion process at the Crude Distillation Unit (CDU) takes place in the crude heaters (furnaces). The main function of the furnace at the CDU is to heat the Crude Oil to attain a temperature of 340 °C at the furnace outlet. Before the Crude Oil enters the furnaces it is preheated in two parallel heat exchangers train where it exchanges heat with Residue, the Middle Distillates and the Pump arounds to a temperature of 200-220 °C.

This process arrangement enhances better process integration, more efficient heat transfers to achieve desired furnace outlet temperature at minimum cost. Thus the duty of the furnace is then limited to heating the Crude Oil from about 220 °C to about 330 -350 °C.

2.2.1 TYPE OF FURNACES

The CDU has two Crude Oil furnaces, which are the horizontal tube cabin type. The furnaces are natural draft, with both radiant and convection heat transfer zones. The furnaces are double pass with Crude Oil following two parallel paths (passes) through the tubes. The crude first enters the convection section and then through the radiant section.

Fig. 4 shows Cabin-Type Furnaces and Fig. 5 also shows Double Pass Furnace.

2.2.2 BURNERS

The burners used in the furnaces are the John Zink low NOx combination type. They are located at the floor of the furnace in the combustion chamber. The burners are vertically (upfire) oriented in one roll. Each of the Crude Oil furnaces has ten (10) burners.

Combined oil and Gas Burner is shown at Fig. 6

2.2.3 FUEL SUPPLY TO BURNERS

There are two (2) types of fuel for the combustion processes at the Tema Oil Refinery. These are:

i. Residual fuel oil that is atomized with medium pressure steam (MPS)
ii. Refinery fuel gas

The main valves that supply fuels to the fuel header of both fuels are pneumatic controlled automatically operated. However, the controls of fuel to the individual burners are separate manually operated valve. When a burner is being fired on residual fuel oil, the atomizing steam
pressure is set automatically at 2.5 bar above the pressure of the refinery fuel oil to the burner. This gives good atomization of the fuel oil and efficient burner performance in the furnace. Fig. 7 shows the Crude Heater Firing Section.

Fig. 4: CABIN - TYPE FURNACE

1 - Burners
2 - Combustion chamber
3 - Radiant section
4 - Convection section
5 - Collector
6 - Stack
Fig. 5: DOUBLE PASS FURNACE

1 - First pass inlet
2 - Second pass inlet
3 - First pass outlet
4 - Second pass outlet
Fig. 6 - Combined Oil and Gas Burner.
2.3.3 COMBUSTION CONTROL

The air for the combustion processes is introduced into the furnaces through primary and secondary shutters on the individual burners. The opening of the shutters are manually adjusted as and when necessary to control the air flow rate into the furnace to maintain the specific excess oxygen (O₂) in the flue gases.

To maintain a balanced draft in each of the furnace a butterfly valve referred to as the furnace damper has been installed in each of the stacks. These are manually adjusted to maintain a constant negative pressure in the furnaces of minus 6.5 mm to minus 12.5-mm water gauge.

3.0 FUELS

As mentioned earlier in Section I, two main types of fuel are burnt in the boilers and furnaces. These are Residual Fuel Oil (RFO) and Refinery Fuel Gas (RFG). The characteristics of the fuels are shown below in tables 1 & 2.

<table>
<thead>
<tr>
<th>Table 1 (Fuel Oil Characteristics)</th>
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<tbody>
<tr>
<td>Flash Point</td>
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<tr>
<td>Specific Gravity</td>
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<tr>
<td>Viscosity at 80 °C</td>
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<tr>
<td>Heating Value(LHV), kcal/kg</td>
</tr>
<tr>
<td>Sulphur % wt</td>
</tr>
<tr>
<td>Ash</td>
</tr>
<tr>
<td>Temperature at burner</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 2 (Fuel Gas Characteristics)</th>
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</thead>
<tbody>
<tr>
<td>Heating value(LHV), Kcal/kg</td>
</tr>
<tr>
<td>Molecular wt</td>
</tr>
<tr>
<td>Hydrogen % vol.</td>
</tr>
<tr>
<td>Methane % vol.</td>
</tr>
<tr>
<td>Ethane</td>
</tr>
<tr>
<td>Propane</td>
</tr>
<tr>
<td>Butane</td>
</tr>
<tr>
<td>Temperature at burner</td>
</tr>
</tbody>
</table>

3.1 FUEL HANDLING

Optimum performance of any burner system can be achieved if combustion fuels, amongst other requirements are properly handled for quality to meet desired specifications.
PART LIST

<table>
<thead>
<tr>
<th>ITEM</th>
<th>Q.TY</th>
<th>DESCRIPTION</th>
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<td>BURHER TILE IN &amp; SECTION</td>
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<tr>
<td>2</td>
<td>1</td>
<td>REGIN TILE</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>SUPPORT REGEN TILE</td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>GAS TIP</td>
</tr>
<tr>
<td>5</td>
<td>4</td>
<td>GAS NIPPLE</td>
</tr>
<tr>
<td>6</td>
<td>1</td>
<td>GAS MANIFOLD</td>
</tr>
<tr>
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<td>1</td>
<td>OIL GUN GUIDE TUBE</td>
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<td>8</td>
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<td>9</td>
<td>1</td>
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<tr>
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<td>ATOMIZER ASS. LY</td>
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<td>1</td>
<td>OIL BODY</td>
</tr>
<tr>
<td>12</td>
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<tr>
<td>13</td>
<td>2</td>
<td>GASKET</td>
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<tr>
<td>14</td>
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<td>PILOT MIXER ASS. LY</td>
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<td>LIGHTING PORT &amp; SIGHTING PORT</td>
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<td>INSULATION 25mm THK</td>
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<td>26</td>
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<td>PRIMARY AIR CONTROL HANDLE</td>
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<tr>
<td>27</td>
<td>1</td>
<td>SECONDARY AIR CONTROL HANDLE</td>
</tr>
</tbody>
</table>

3.3 RESIDUAL FUEL OIL

Residual fuel oil that is the heaviest fraction in the distillation process is stored in 8 tanks. Two of the tanks- G31 & G32 are designated for storing Residual fuel Oil for combustion in the boilers and furnaces. There are steam heating coils in the tanks, which maintain the fuel temperature between 50 - 60°C for easy pumpability. One tank is put into service at a time. The out of service tank is replenished and drained at regular intervals to get rid of condensate (water) before it is put in service. The fuel oil piping from the tank to the boiler / furnace is through a pump and has inline heat exchanger to regulate the fuel oil temperature and filters /strainers to rid the oil of any solid particle before the oil reaches the burners. Fig. 8 shows Residual Oil Train.
Case Study
3.3 REFINERY GAS

Refinery fuel gas which is the lightest fraction in the distillation process is piped into an accumulator/knockdown vessel. From the vessel the gas is distributed to the boilers and furnace. The gas before entering the boiler or furnace is thoroughly drained of any condensate. Gas separators to knock out any condensate still entrained in the gas flow are installed in the gas circuit further down stream. Fig 9 shows the Refinery gas train.

3.4 ECONOMIC APPLICATION OF FUELS

The operating situation at the process plant at any particular time determines the quality and quality of refinery fuel available for combustion. When the Crude distillation unit alone is in operation, limited quality of gas (without hydrogen) is available and the percentage fuel oil combustion is higher than that of gas. However, if the Premium former unit is also in operation, sufficient gas (this time with hydrogen) becomes available and the percentage fuel gas combustion is higher than that of oil. The economic consideration is always to burn more gas than oil depending on its availability at any given time.

4.0 COMBUSTION AND BURNER MANAGEMENT SYSTEMS TECHNIQUES.

THEORY OF COMBUSTION

Combustion is rapid break down and recombination of combustible compounds with oxygen and the liberation of heat as a result of this process.

The ultimate objective of any fuel burning system is to obtain the maximum amount of heat (energy) from the smallest quantity of fuel (highest thermal efficiency), while maintaining required air emission standards.

The major components of fuel are carbon, hydrogen, and oxygen. Small quantities of other components such as sulphur, nitrogen, metals, ash, etc. may also be present. Air is composed of a mixture of oxygen and nitrogen with trace quantities of carbon dioxide, water vapour, and other relatively inert gases. For practical purpose the trace quantities of inert gases can be ignored and dried air considered to be a mixture of 21% oxygen (entering as O₂) and 79% nitrogen (entering as N₂) by volume.

Every fuel requires a specific amount of oxygen to complete the reaction of carbon to carbon dioxide, and hydrogen to water: This amount is referred to as 'stoichiometric' oxygen requirement. When less than this theoretical amount of oxygen is added the reaction is said to be proceeding under sub-stoichiometric conditions. Sub-stoichiometric combustion results in unburned fuel and the formation of carbon, hydrocarbon combustibles and/or carbon monoxide.

However, even perfectly stoichiometric combustion results in some unburned fuel due to the inability of any burner system to "perfectly" mix the fuel in air and the combustion process.
Consequently, it is necessary to add more oxygen (in air) than is "stoichiometrically" required for combustion. This additional air is called "excess air". It is important that only enough excess air be added to ensure complete combustion, since any additional air reduces boiler efficiency. Any gases, which are not directly participating in the combustion process (that is anything but the fuel and stoichiometric amount of oxygen), will absorb heat from the combustion process. When these gases exit the stack at a temperature higher than ambient temperature, they take with them some of the useful heat generated in the combustion process. This is known as the "dry" stack gas loss which, amongst other losses, is used in determining boiler efficiency.

The total amount of heat liberated during the burning of a fuel is referred to as the "heat of combustion", and is the sum total of each of the component parts of the fuel. Hydrogen, when combined with oxygen to form water in the burning process, liberates 62,00 BTU's of heat per pound (68,317 cal/mole). Carbon liberates 14,540 BTU's per pound (94,052 cal/mole) when converted to CO₂. However, when insufficient oxygen is present to complete the reaction of carbon + CO₂, Carbon monoxide is produced. Carbon monoxide formation liberates 4,440 BTU's per pound (67,636 cal/mole), i.e. a net loss of heat production of 10,000 BTU's per pound compared to carbon dioxide. It is obvious, therefore that it is essential to provide sufficient excess air to complete the combustion process, while at the same time minimizing excess air to maximize boiler efficiency.

4.1 CONCEPTS FOR BURNER DESIGN

Controlling the quantity of excess air to ensure complete combustion is, however only a part of the requirement. The burner system must also control the method in which the fuel is prepared for combustion, the speed and direction of fuel injection, and how the fuel mixes with the combustion air. These concepts form the basis of each manufacturer's burner design. The heating value of the fuel can be expressed either as higher heating value (HHV) or "Lower Heating Value" (LHV). Either value is correct and acceptable, but it is essential that the heating value be correctly expressed.

HHV assumes that the water vapour formed during the combustion process condenses and gives up this heat of condensation to the process; LHV assumes no water vapour condensation. It is most common to express the heating value as HHV. When this is the case, the boiler manufacturer takes into account the fact that water vapour does actually condense by reducing the boiler thermal efficiency accordingly, which is accepted approach to calculating thermal efficiency. What is important, however is that no "double dipping" should occur; that is a lower heating value is used, and the boiler manufacturer also accounts for the same loss in his thermal efficiency calculations. When this happens, the projected fuel usage is erroneously too high, resulting in an oversized fuel supply system.

One other important consideration is that even with excess air and adequate mixing, the combustion process can prematurely interrupted by flame impingement on the furnace walls or exit tubes. When this happens, the combustion reactions are slowed or stopped by the lowering of
the temperature in this region, thereby effectively "quenching" any further combustion. This creates the same effects as inadequate air and must therefore be avoided.

One final factor to be considered when designing any burner system is that any air that does not enter the furnace through the burner system will result in a loss in efficiency and higher excess air requirements. The burner is the only device designed to mix fuel and air for the combustion process; any air not entering through the burner will not be properly mixed, thereby raising the minimum oxygen requirement.

4.2 NOₓ FORMATION AND CONTROL

The formation of NOₓ during the combustion of fossil fuel has been associated with two distinct mechanisms generally referred to as "Thermal NOₓ" and "Fuel NOₓ". Thermal NOₓ refers to the NOₓ generated by the high temperature reaction of atmospheric nitrogen and oxygen present in the combustion air. Thermal NOₓ is highly temperature dependent since high energy is needed to break the nitrogen molecule's chemical bond. Fuel NOₓ is formed by the oxidation of organically bond nitrogen in fuel during combustion. Fuel NOₓ is less sensitive to flame temperature than Thermal NOₓ (since less energy is required to free up the nitrogen atom) but is strongly influenced by oxygen availability.

Combustion techniques available to reduce NOₓ emission include:
1. Low excess air operation
2. Staged combustion (off-stoichiometric firing)
3. Flame temperature reduction
   (a) Flue gas re-circulation
   (b) Air preheat reduction
   (c) Re-circulation flue gas temperature reduction

4.3 FLAME CONSIDERATION FOR OIL FIRING

Optimum air velocities and proper atomization pressure are required to produce the turbulence and droplet size necessary for correct air and oil mixing, flame shape, and stability. If insufficient air is being used or if the atomization pressure is insufficient, black smoke will form and the boiler may tend to pulsate or flutter. Under these conditions, the flame will be seen to swell and assume a dark orange to red colour.

An excess of air will cause the formation of white or brown smoke, and when the flame is viewed, it will appear to be ragged with sparks appearing at the edges. In particularly bad cases of high excess air, unburned oil droplets will be torn away from the main flame and deposited on the furnace lining and boiler surface. The white and brown smoke is normally the result of a "chilling" of the flame by the high excess air. It may also be the result of flame impingement on the walls of the boiler, which similarly results in the "chilling" of the flame. A flame that in general appears to have the proper geometry and colour, but which exhibits a high level of
sparklers or oil drops is likely the result of inadequate atomization, or when steam is the atomizing medium, "wet steam". When a burner is operated below the lower end of an acceptable turndown range, the flame will also be ragged in appearance and will lose its normally well-defined shaped. White smoke will be produced as result of the "chilling" of the flame by excess air, but black smoke may also be present due to the poor mixing of the oil droplets and air. Increasing the atomizing media pressure may help in correcting this condition, but a turndown level will be reached where no further change in operating conditions will be successful. At this level, the minimum turndown has been reached for that particular burner/boiler configuration. Increasing the airflow will further chill the flame; decreasing the airflow will result in incomplete combustion. Under such conditions, increasing the fuel flow until acceptable conditions are met may be necessary.

4.4. IMPORTANT COMBUSTION CONTROL TIPS

On first igniting an oil fire, it will be necessary to input fuel at a rate in excess of the turndown minimum. This is true because the limits of flammability for igniting a fuel are much narrower than when the flame has already been established. Burner management and combustion control systems must be designed to allow discrimination between these "low-fire light off" and "minimum fire" requirements. Under normal operating conditions when burning fuel oil there should be no difficulty in obtaining a very good flame over a fairly wide range of atomizing media pressure. To obtain the best combustion conditions at normal operating loads while maintaining proper flame supervision, the following steps are performed:

1. View the flame in the furnace. It should not be touching any of the boiler walls or tubes, and it should be symmetrical around the burner. The flame must attach to the atomizer nozzle within a distance corresponding to ½ the swirler diameter, and must not pulsate.
2. If all the conditions in 1 are met, and black smoke still exits, the burner atomizer media flow must be raised until no smoke is visible. If this is unsuccessful, raise the burner airflow until the black smoke disappear. If white smoke is present, reduce the burner airflow until the smokes disappear.
3. View the flame in the furnace—it should be of a bright white orange colour.
4. From minimum fire to maximum fire, the flame appearance will generally have the following characteristics:
   a) Minimum fire to 30% firing rate(load). The fire will be bright yellow with distinct spokes corresponding in number to the number of atomizer nozzle orifices. The center of the fire will be clean, and it will be possible to view the primary combustion zone swirl. The fire will be short and of a diameter slightly larger than the quad opening.
   b) 30% to 60% Firing Rate. Though it will be possible to distinguish individual atomizer jets, the center of the flame will have dirty wisps, and the central area will lengthen considerably. The diameter will also increase somewhat, but not as significantly as the length. The colour of the fire will tend more toward orange, except for the central area which will appear brownish.
   c) 60% to 100% Firing Rate. The outer region of the flame will bend significantly and envelop the center region. The brownish center will therefore be no longer apparent. The flame length
will be only slightly longer than that viewed in the 30% - 60% firing rate range. The colour will remain yellow. The colour will remain a yellowish orange.

5.0 OIL ATOMIZATION PRINCIPLES

5.1 VISCOSITY

To effectively burn fuel oil, the oil must be broken down into very small droplets so that effective intermixing with air is possible. To accomplish this, the fuel oil must be at the proper viscosity to permit thorough atomization. For most fuels, heating is required to lower the viscosity to an acceptable level. Once the fuel is at the proper viscosity it must be atomized in the most effective manner.

Fig. 10 shows the variation in viscosity with temperature for typical fuel oils. The viscosity of most oils are stated in Saybolt Seconds Universal (SSU) at 100°F for reference. This reference point is noted for all of the oils on the chart by slanted lines. If the viscosity of any particular oil does not correspond with an exact value on the chart, an additional curve (line) may be interpolated to suit that particular oil. Two additional lines have been added to the chart to show the ideal range of viscosity for atomizing the oil in a number of atomizer designs. By following the slanted viscosity line of the particular oil to be used until it intersects with the two horizontal lines, the range in temperature for optimum atomizer can be determined. The viscosity of TOR's fuel oils is determined at 50°C.

5.2 STEAM/AIR ATOMIZATION

For cold start where steam is not available, dry compressed air at approximately 80-100psig can be used with dual fluid atomizers. During normal operation, steam atomization is preferred. Atomizing steam must be dry.

At maximum load conditions it is normally desirable to atomize at the highest possible steam pressure to achieve the smallest possible droplets. At low fire conditions, however, the optimum steam pressure is a compromise; high pressure is too high and low pressure is too low to maintain a stable flame. The final steam pressure is a compromise between the high pressure required for large load requirements and the requirements at smaller load requirements varying from a minimum of 80 psig to a maximum of 150 psig. Up to 180 psig atomising steam pressure is available for the burners at TOR.

The maximum oil pressure should be limited to that pressure which will allow the maximum firing rate to be achieved. The oil flow control valve provides the required oil flow at lower firing rates.
5.3 **FLAME MONITORING SYSTEM**

Three flame scanner heads are fitted per burner/register.
1. Ultra-violet type UV, MK II scans the pilot/ignitor gas flame. (Fig. 11)
2. Infrared I.R. 800 Mk II scans main oil burner flame. (Fig. 12)
3. Ultra-violet type UV MK II scans main gas burner flame.
Fig. 11 — SECTION THROUGH UV 2 FLAME SCANNER HEAD
Fig. 42. — SECTION THROUGH I.R. FLAME SCANNER HEAD TYPE I.R.808
5.4 MONITORING

Separate 'Dualscan' flame-monitoring units are used for the pilot and main burner flame detection systems. The flame monitoring and detection provides both infrared (IR) and ultra-violet (UV) scanning within a single control unit. Separate connections allow for the use of IR 800 and UV MK II flame viewing heads.

The 'Dualscan' unit front facia in fig 13 incorporates two L.E.D. bar graphs. The left-hand graph gives continuous appreciation of the IR or UV flame signal (whichever is greater) with reference to the threshold setting (set by thumbwheel) displayed on the right hand graph. Three L.E.D indicators on the upper left-hand side of the front facia indicate FLAME ON, HEAD FAULT and SYSTEM FAULT CONDITIONS.

A head fault or system fault condition, irrespective of the system (IR or UV) on which it occurs or which system is monitoring the stronger flame currently, will cause a flame off condition to be indicated.

5.5 DUALSCAN SYSTEM WITH VIEWING HEAD IR 800 MK II -DESCRIPTION

The system consists of the Dualscan, interconnecting cable and Solid State viewing head, which detects presence of various types of flame and can operate in hazardous areas at temperatures up to 85 °C.

5.6 OPTICS

A 25mm diameter glass lens and 40mm focal length is used to focus light on to a photovoltaic diode detector which generates its own power from the incident light. The lens increases the light intensity at the detector by a factor of 20 and narrows the field of view to approximately 4.5 °, which improves spatial discrimination.

5.7 DUALSCAN SYSTEM WITH VIEWING HEAD UV MK II VIEWING -DESCRIPTION

The system consists of the Dualscan, interconnecting cable and UV MK II viewing head. The detector used is an ultra violet sensitive photocell, which conducts when energized by electromagnetic radiation of suitable wavelength, provided that a high voltage is present across its electrodes. It is responsive to radiation in the wavelength 150 to 250 nm, which is near ultra violet, just beyond the range of human vision.
Fig. 13  DUALSCAN  FRONT FACIA
5.8 OPERATION

UV cell pulses pass through the cell latch, which allows no more than one pulse per half cycle. If a head fault or system fault occur, the latch circuit can be reset after correcting the fault by pushing the reset bottom on the front facia. The system is electronically self-checking, enable the three failure modes of the UV cell to be detected i.e.

i. Open circuit, which gives no signal input and hence flame off condition.
ii. Short circuit, which will give maximum input signal and hence a fault condition.
iii. Soft cell (defined a cell which strikes every half cycle of the mains, regardless of whether or not it is being energized by UV radiation) which will also give a maximum input signal and hence cause a fault condition to flash up.

NOTE:

To prevent condition (III) being wrongly detected when high levels of UV radiation saturate the photocell, an interrupter vane assembly is fitted to the detector head. The width and speed of the vane have been calculated to block off radiation to the cell for at least one complete half cycle of the supply voltage in every second. Therefore the pulse counter can never reach 99 when the cell is driven by an external UV signal.

If the vane should stop turning for some reason the system will always fail-safe. If the vane stops in front of the cell a flame off condition will occur. In any other position the Digiscan will either work normally or go to FAULT, depending on the UV level received by the cell.

6.0 SAFE COMBUSTION PRACTICES

All burners at TOR have been designed to meet the criteria and recommendation of the National Fire Protection’s Association’s (NFPA) standard 8501. TOR therefore endeavors to operate the burners in accordance with this standard. The specific instructions for the safe operation of the Burner Management System as well as other safety measures accompanying the combustion equipment are highlighted in the instruction manual of the equipment. All measures affecting operator safety are of equal importance at all times. Operator’s attention is always drawn to the specific WARNING OR PRECAUTION pages in the Instruction manual.
These include:

**TITLE**

Explosives
Boiler Purge
Hazards of sub-stoichiometric combustion
High Energy Ignitor Unit
Gas Ignitor
Ultra-Violet Flame Monitoring Head
Safety Interlock-Routine Checks
Windbox Inspection
Infra Red Scanner Hot Refractory Hold In

**PURPOSE**

Warning

Precaution

Precaution

6.1 FUTURE EXPECTATIONS OF TOR

At present, two additional boilers are being installed to support the foreseen increased steam demand in the refinery. One is 35 ton/hr and the other 60 ton per hour. The steam quality and specification are same as the three boilers mentioned earlier. All contract agreement for the installation of a fluid catalytic cracking unit have been concluded and the project has kicked off.

6.2 ENVIRONMENTAL MANAGEMENT

**OUTLINE**

- Environmental Policy
- Potential Releases
- Potential Operational Releases
- Monitoring Program for Actual Emissions

Environmental Policy

The Tema Oil Refinery seeks to refine crude oil into various petroleum products in such a way that substances released would have minimum or non-significant impact on air, water and land. ‘Because the company has a strong regard for environmental protection, product stewardship and safety concerns’, our objectives are:

- To incorporate the Best Available Environmental Techniques not entailing excessive cost
- To maintain and operate existing pollution control equipment to ensure maximum recovery, reuse and/or recycle
- To improve and operate effectively and efficiently existing contingency plans for oil spillage, fire and explosion
- To maintain close and good working relationship with emergency response agencies for oil spill, fire and explosion in the local community and region
To be both responsible and responsive in our efforts relating to environmental protection, product stewardship and employee safety

The Tema Oil Refinery (TOR) Ltd. is a simple Hydroskimming Plant with a capacity of million tons consisting basically of:

(a) Atmospheric Crude Distillation Unit
(b) Catalytic or Premium Reforming Unit

The potential atmospheric releases due to the various stages of TOR's production processes particularly burning of fuel oil and fuel gas include:

(a) Gaseous emissions such as:
   - SO\textsubscript{X}
   - NO\textsubscript{X}
   - CO
   - Volatile organic compounds (VOC)

(b) Atmospheric Particulate
   - Total suspended Particulates (TSP)
   - Inhalable Particulates (PM\textsubscript{10} & PM\textsubscript{2.5})

The furnace has no existing air pollution control device, except the stacks ranging from a height of 30M to 50M for the dispersion of smoke and other air pollutants associated with combustion.

The Potential Operational air emissions that are those emissions that the unit is capable of producing in the absence of any permitted restrictions are:

Fuel Gas Analysis of Residual Fuel Oil (RFO) and Refinery Fuel Gas

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Fuel Gas</th>
<th>Fuel Oil</th>
</tr>
</thead>
<tbody>
<tr>
<td>O\textsubscript{2}</td>
<td>869</td>
<td>1,222</td>
</tr>
<tr>
<td>N\textsubscript{2}</td>
<td>22,077</td>
<td>24,272</td>
</tr>
<tr>
<td>CO\textsubscript{2}</td>
<td>4,169</td>
<td>6,010</td>
</tr>
<tr>
<td>H\textsubscript{2}O</td>
<td>3,237</td>
<td>2,852</td>
</tr>
<tr>
<td>SO\textsubscript{X}</td>
<td>4.53</td>
<td>41.3</td>
</tr>
<tr>
<td>NO\textsubscript{X}</td>
<td>5.00</td>
<td>12.09</td>
</tr>
<tr>
<td>Particulates</td>
<td>0.29</td>
<td>5.39</td>
</tr>
<tr>
<td>CO</td>
<td>0.61</td>
<td>1.72</td>
</tr>
<tr>
<td>Excess air</td>
<td>15 %</td>
<td>20 %</td>
</tr>
</tbody>
</table>

Combustion Diagnostics and Optical Techniques
The permitted allowable emissions in the form of standards/Regulations from EPA are as follows:

<table>
<thead>
<tr>
<th>NO</th>
<th>SUBSTANCE</th>
<th>TIME WEIGH AVERAGE, (TWA)</th>
<th>AVERAGE TIME</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Sulphur Dioxide (SO₂)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Industrial 900µg/m³</td>
<td></td>
<td>1 hr.</td>
</tr>
<tr>
<td></td>
<td>Residential 700µg/m³</td>
<td></td>
<td>1 hr.</td>
</tr>
<tr>
<td></td>
<td>Industrial 150µg/m³</td>
<td></td>
<td>24 hrs.</td>
</tr>
<tr>
<td></td>
<td>Residential 100µg/m³</td>
<td></td>
<td>24 hrs.</td>
</tr>
<tr>
<td></td>
<td>Industrial 80µg/m³</td>
<td></td>
<td>1 yr.</td>
</tr>
<tr>
<td></td>
<td>Residential 50µg/m³</td>
<td></td>
<td>1 yr.</td>
</tr>
<tr>
<td>2</td>
<td>Nitrogen Oxide (Measured as N)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Industrial 400µg/m³</td>
<td></td>
<td>1 hr.</td>
</tr>
<tr>
<td></td>
<td>Residential 150 µg/m³</td>
<td></td>
<td>1 hr.</td>
</tr>
<tr>
<td></td>
<td>Industrial 60 µg/m³</td>
<td></td>
<td>24 hrs.</td>
</tr>
<tr>
<td></td>
<td>Residential</td>
<td></td>
<td>24 hrs</td>
</tr>
<tr>
<td>3</td>
<td>Total Suspended Particulate (TSP/SPM)</td>
<td>230 µg/m³</td>
<td>24 hrs.</td>
</tr>
<tr>
<td></td>
<td>Industrial 150µg/m³</td>
<td></td>
<td>24 hrs.</td>
</tr>
<tr>
<td></td>
<td>Residential 75µg/m³</td>
<td></td>
<td>1 yr.</td>
</tr>
<tr>
<td>4</td>
<td>Carbon Monoxide (CO)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Industrial 100 mg/m³</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>60 mg/m³</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>30 mg/m³</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>10 mg/m³</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

In pursuance of TOR’s environmental policy and in compliance with the national environmental guidelines and statutory requirements an environmental air quality assurance is being established through:
The development of an environmental monitoring system and programme that outlines sampling sites, protocols for sampling, sampling preparations and analysis

- Developing the capacity for predicting atmospheric pollution through plume modeling techniques
- Generating data and information at the baseline and prevailing levels on the air pollutants of interest: SOx, NOx, CO, CO2, TSP, PM_{10}, PM_{2.5} and elemental analysis.

The monitoring is being carried out in three phases:

a) PHASE I

**Sampling Sites**
Five sampling sites in and around the refinery have been chosen for the prevailing levels and four sites for the baseline levels. These were chosen based on the following:

- a non-industrial area with little vehicular traffic flow
- relative proximity to the project site
- possible effect of anthropogenic and natural sources

**Plume Modeling**
Very little capability exists in the local private or public sector for the air quality prediction through plume modeling.
The inputs into the plume modeling software program will include:
- prevailing meteorological conditions (to be used for atmospheric stability class determination)
- source emission profile

b) PHASE II

**Baseline Level Monitoring Program for Background**
A 24-hour sampling will be done for all sampling sites (four sites) for the analysis of Total Suspended Particulates (TSP) through Gravimetric analysis of loaded filters, the analysis of SOx, NOx, CO and CO2 through the use of a direct reading gas monitor deploying the use of diffusion barrier technology (electrochemical fuel cell sensor)

c) PHASE III

Gravimetric analysis of loaded filters and the Direct Reading of the gaseous pollutants through electrochemical fuel cell sensors of all 24-hour samples will be done for the air quality assurance of the five sampling sites chosen from in and around the refinery.
6.3 RESULTS

Airborne Particulate Matter
One type of air sampler has been used in monitoring airborne particulate matter: Sierra Andersen constant flow air sampler, with TSP filter head.

Total Suspended Particulate Matter Results

<table>
<thead>
<tr>
<th>Sampling Site</th>
<th>Time Weighted Average, ug/m³ (24 hr)</th>
<th>EPA Guideline (24 hr,</th>
</tr>
</thead>
<tbody>
<tr>
<td>GAEC.RTC</td>
<td>14.0</td>
<td>150</td>
</tr>
<tr>
<td>DOME.TL</td>
<td>264.0</td>
<td>&quot;</td>
</tr>
<tr>
<td>DOME.ST</td>
<td>200.0</td>
<td>&quot;</td>
</tr>
<tr>
<td>UPVALE</td>
<td>120.0</td>
<td>&quot;</td>
</tr>
</tbody>
</table>
From the sites sampled, TSP values ranged between 14.0 – 264.0 ug/m³ with an average of 149.5 ug/m³. Compared to ambient air quality guidelines from EPA of 150.0 ug/m³, the sites sampled are just within the guidelines.

The Atmospheric Environment
The meteorological conditions prevailing in the background area and the refinery has been summarized in Figure 14 and 15 for the following:

- mean temperature
- mean rainfall
- mean number of sunshine hours
- windspeed

The meteorological data will be used to determine the stability class, which is an input in software model.

SOME CONTROL MEASURES UNDER PRACTICE

- Low Sulphur fuel oil for combustion
- Floating Roof Storage Tank
- Pressurized Tanks
- Vapour Recovery System
- Accumulator Vents
- Specific Colors for Storage Tanks
Fig. 14 PLOT OF MONTHLY MEAN ATMOSPHERIC PARAMETERS
7.0 RECOMMENDATIONS

The workshop should recommend the type of laser/optical techniques for the measurement of pollutant parameters that lend themselves to laser-based diagnosis.

2. BRIEF OVERVIEW OF PROCESSES AT TOR

3. COMBUSTION SYSTEMS
   - BOILERS
   - FURNACES

4. FUELS
   - FUEL HANDLING
   - FUEL CHARACTERISTICS

5. COMBUSTION AND BURNER MANAGEMENT TECHNIQUES

6. FLAME CONSIDERATIONS OF OIL FIRING

7. OIL ATOMISATION PRINCIPLES
   - VISCOSITY

8. FLAME MONITORING SYSTEMS

9. SAFE COMBUSTION SYSTEMS

10. ENVIRONMENTAL POLICY

**NO**\(_X\) FORMATION AND CONTROL

- THERMAL NO\(_X\) – TEMPERATURE DEPENDENT
- FUEL NO\(_X\) – OXIDATION OF ORGANICALLY-BOUND NITROGEN IN FUEL DURING COMBUSTION

TECHNIQUES TO REDUCE NO\(_X\)

- LOW EXCESS AIR
- STAGED COMBUSTION
(OFF-STOICHIOMETRIC FIRING)

- FLAME TEMPERATURE REDUCTION
  - FLUE GAS RECIRCULATION
  - AIR PREHEAT REDUCTION
  - RECIRCULATION FLUE GAS
  - TEMPERATURE REDUCTION

7.1 COMBUSTION CONTROL
The boilers are equipped with forced-draft fans with electric and steam-turbine drives. Combustion air-flow is automatically operated and controlled by inlet guide vanes, which are pneumatically actuated remotely. The air registers are normally fully open.
CASE STUDY ON COMBUSTION PROCESSES IN THERMAL PLANT AND ENERGY GENERATION - TAKORADI THERMAL POWER PLANT

STEPHEN KWAKYE DOKU
TAKORADI THERMAL PLANT
P. O. BOX M77
TEMA, GHANA

1.0 INTRODUCTION
The Volta River Authority (VRA) was established under the Volta River Development Act 1961 (Act 46). Its primary functions are the generation of electric power, transmission of electric power and since 1987 distribution of electric power.

The power generation system in Ghana, until December 1997 was dominated by two hydroelectric plants, Akosombo Generating Station, with an installed capacity of 912 MW and Kpong Generating Station with installed capacity of 160 MW. Figure 1 shows the VRA system.

The long term average inflow into Lake Volta is 1196m$^3$/s. An important characteristic of the hydrology of the Volta basin, however, is the extremely high variability from year to year. To illustrate this, the highest recorded annual inflow is 3084m$^3$/s, while the lowest is 242 m$^3$/s i.e. the maximum is 13 times as large as the minimum. Figure 2 illustrates the mean annual inflow rates from 1936 to 1998. In addition to the high variability from year to year, the recorded flows from the Volta River demonstrate that it is common to have prolonged wet and dry periods lasting over a decade.

On the average, the potential energy available from the two hydroelectric power plants is estimated to be 6000 GWh/yr. However, the energy yield is relatively low over the prolonged droughts occasionally experience in Ghana. Simulations indicate that the energy yield in the dry years would be as low as 4800 GWh/yr over the 41/2 year long depletion period for Lake Volta. Conversely, during the cycle of wet years, the energy yield can be as high as 8000 GWh/yr with a significant volume of water passed through the spillways without generating power.

Operation of the hydro system required that the Volta Lake be retained at relatively high levels to be prepared in the event of a prolonged dry period. This results in maximization of the firm energy yield from the developments. The disadvantage of this necessary approach is the excessive spillage of water would occur if a prolonged wet period were to occur instead. It is estimated that over the long term, 13% of the potential energy would be spilled.

2.0 PLANNING STUDIES
In the 1970's and 1980's a prolonged drought was experienced in Ghana and it became apparent that the existing hydroelectric facilities had less energy than was earlier estimated. Acres International Limited (Acres) were therefore contracted in 1983 to conduct a comprehensive generation and transmission planning study to provide VRA with master plan for the orderly and economic expansion of those facilities. It was to identify both the specific projects that should be undertaken in the short term to meet anticipated growth in electrical power demand in Ghana and the general direction that such expansion should take over the next 20 years.
The study, conducted over an 18 month period, determined that future generation expansion could be by development of some part of the hydro resources, in which case the reservoir operating policy would not be changed. Alternatively, is could be based on thermal generation, in which case the operating strategy could be changed, reducing spillage to 3%. In the latter case, about 600 GWh/yr of additional hydro energy would become available from Akosombo and Kpong. The increment of otherwise lost hydro energy would be obtained with a relatively low capital investment in thermal plant operated on a base-loaded mode but in only approximately 1 out of 7 years and therefore with low average fuel costs.

The study indicated that the present-worth capital and operating costs for mixed hydro-thermal generation expansion schemes are significantly lower than all hydro schemes. The recommended development plan over the following 20 year period comprised 50 MW Combustion Turbine Plant followed by 300 MW of steam plants.

A study conducted jointly by VRA and ACRES in 1986 updated the earlier plan and confirmed the positive economics of a thermal-based development plan over the next 20 years. There was an update in 1987. In 1992, the thermal plant feasibility study optimised the development to a 600 MW combined cycle plant comprising of 2 sets of 2 combustion turbines, associated Heat Recovery Steam Generators and Steam Turbine Configuration (Figure 3). In addition there was to be transmission system expansion to evacuate the power produced. A second part of the feasibility study stied the plant at its present location of Abobade.

3.6 IMPLEMENTATION PROJECT

Based on further analysis and as a result of discussions with the World Bank in June/July 1993, the project was re-dimensional to a 300 MW Combined Cycle Plant.

The project is being implemented as the Takoradi Thermal Power Project.

3.1 PROJECT DESCRIPTION

The main components of the project are:

1. Combined Cycle Plant
2. Associated Transmission Lines

The 300 MW combined cycle generating plant was to have dual firing capability to burn Light Crude Oil as well as natural gas. The fuel oil was to be supplied through a dedicated marine tanker unloading facility and connecting pipeline.
3.2 CONTRACT PACKAGING

The Takoradi Thermal Power Project is divided into 8 main contract packages, namely:

Contract TK - 1: Combustion Turbine and Site Development.
Contract TK - 2: Steam Turbine and Heat Recovery Steam Generators (HRSGs)
Contract TK - 3: Management and Operation of the Takoradi Thermal Power Station and Training and Development of Owner's Personnel
Contract TK - 4: Consultant's Services for Project Implementation.
Contract TK - 5: Township Development
Contract TK - 6: Transmission Line and Substation Modifications.
Contract TK - 8: Marine Investigations.

ACRES provided the consultancy services up to the Contract Negotiation of Contract TK-1.

3.3 ENVIRONMENTAL ASSESSMENT

A detailed environmental assessment report entitled: "Takoradi Plant, Environmental Impact Assessment" was prepared by ACRES. The report contains, among others, the existing natural and social setting, and the potential impacts and measures proposed to mitigate and/or monitor these impacts in accordance with environmental requirements of the funding agencies. A detailed pre-construction and post-construction programme, covering physical and biological characteristics of local marine environmental, terrestrial ecology of the site and transmission corridor, ambient site air quality and noise levels were defined for implementation.

3.4 PROJECT FINANCING

The total cost of the project was estimated as US$411.90 million.

Funding for the project is as follows:

1. International Development Agency (IDA) - 42.63%
2. European Investment Bank (EIB) - 11.29%
3. Commonwealth Development Corporation (CDC) - 4.80%
4. CaisseFrançaise de Développement (CFD) - 7.28%
5. Kuwait Fund for Arab Economic Development (KFAED) - 5.34%
6. Arab Bank for Economic Development in Africa (BADEA) - 2.43%
7. Volta River Authority - 2.08%
8. Others - 1.39%

The expected cost to completion is estimated to be about US$ 350 million.
The cost of the power plant component to completion is expected to be US$207 78 million.
4.0 STATUS OF PROJECT

Contract TK-1:
The contract was won by General Electric of USA and became effective on January 1. The first Combustion Turbine started commercial operation on December 32, 1997, while Unit 2 started on January 7, 1998. The balance of plant and other facilities are almost complete and takeover is imminent.

Contract TK-2:
The Contract Agreement between VRA and GE was signed on April 3, 1997 and became effective on April 10, 1997. Commissioning of the Heat Recovery Steam Generators and Steam Turbine is in progress.

Contract TK-3:
The Contract for the Management and Operation of the Takoradi Thermal Power Station and Training and Development of Owner's Personnel, signed between VRA and Electricity Supply Board International (ESBI), became effective on June 4, 1997. It is expected to be completed by June 30, 2000.

Contract TK-4:
The Consultant's Services for Project Implementation contract which was won by Mott Ewbank Preece of the United Kingdom, became effective on September 21, 1995 and is expected to be completed by September 1999.

Contract TK-5:
Contract packages under the Township Development are at various stages of completion and the township occupied.

Contract TK-6:
All the contract packages under the Transmission Line and Substation Modifications are complete. A later addition of Optical Ground Wire (OPGW) on the Aboadze-Prestea line is yet to be completed.

Contract TK-7:
This contract is made up of various packages. VRA is to provide a compensation package to the local communities of Aboadze, Abuesi and Dwomo for the land acquired for the project. The Package includes cash compensation for crops on the acquired land and the provision of social amenities. They are in various stages of implementation.

4.1 Contract TK-8:
The marine investigation contract, which was executed by Hydro Soil Services of Belgium was completed in January, 1995.
Plant Description

Figure 4 shows the layout of the Takoradi Thermal Power Plant. Fuel is received at a Single Pont Mooring (SPM) 4.5 km offshore and pumped into Raw Fuel Tanks. The fuel is treated in the fuel treatment building and stored in treated fuel tanks from where it is forwarded to the turbines for firing.

Water from Ghana Water Sewage Company and the Desalination Plant is received into a reservoir and demineralized for use as water injection for NOx control and make-up water for the Steam Turbine.

Waste heat from the Exhaust of the combustion turbine is used in the HRSG to produce steam for the Steam Turbine. Figure 5 is a schematic diagram showing the process. Condenser cooling water is supplied by the closed cooling system utilizing a cooling tower. Make-up water for the cooling tower is supplied by a 1.5 km seawater pipeline.

5.0 GAS TURBINES

The installed combustion turbines are GE Frame 9E heavy-duty Gas Turbines with an output of 110 MW each. Figure 6 shows a cross section of the Gas Turbine.

Air at atmospheric pressure is admitted into the inlet guide vanes of the Axial Flow, 17 Stage compressor and compressed to 10.58 bar. Fuel is introduced into the combustor where it is ignited. The compressed air support the combustion as well as provide cooling for the combustion liners. The hot gas then flows into the turbine section.

Work is extracted in the turbine from the high pressure, high temperature working fluid as it expands down to atmospheric pressure.

6.0 COMBUSTION IN THE GAS TURBINE

(a) Flame Temperature and Stability

Combustion takes place in the combustor when a stream of atomized fuel or gas is ignited. Flame stability and temperature depends on the fuel to air ratio. The ideal condition is a ratio of 1, i.e. equal volumes of Fuel and Air being burnt. At a ratio of less than 1, the flame stability is poor while the temperature is lower. At fuel to air ratio's greater than 1, then the flame temperature reduces and the flame becomes less stable. Figure 7 shows the relationship between flame temperature and the fuel/air ratio.

Because of the temperature limitations of the materials used for construction of the combustor and the hot gas path parts, it is not possible to allow the flame to achieve the full temperature. The Fuel/Air ratio is therefore less than 1 producing a flame temperature of about 1600°C.

The combustor is designed to allow just enough air to provide flame stability in the critical region before the rest is allowed in downstream. Part of the air is used for cooling of the combustor before joining the stream. By the time it gets to the first stage nozzle through the
transition piece, the gas is cooled to about 1050°C. The gas is then expanded through the three (3) turbine stages and exhausts at a temperature of 560°C.

b) **Products of Combustion**

Combustion of fuel in the Gas Turbine produces the following:

(i) **Carbon Dioxide (CO₂)**
Carbon Dioxide is a product of complete combustion of carbon in the fuel.

(ii) **Carbon Mono Oxide**
Carbon Mono Oxide as a product of incomplete combustion of carbon. The reasons for the situation are high Fuel/Air Ratio and Low Combustion temperature.

(iii) **Oxides of Nitrogen (NOₓ)**
Production of oxides of Nitrogen are temperature related. The higher the temperature, the higher the amount of NOₓ produced.

(iv) **Sulphur Dioxide and Oxides of Sulphur**
Fuel bound sulphur is the source of oxides of sulphur the exhaust gases.

(v) **Particulates**
Particulates are produced by the incombusible parts of the fuel.

### 7.8 IMPACT ON THE ENVIRONMENT

a. **Carbon Dioxide**

CO₂ is one of the “greenhouse” gases and increased levels in the atmosphere have been linked to global warming. It is not possible to predict the exact contribution of specific emissions to these global warming. It is not possible to predict the exact contribution of specific emissions to these global concerns. However, minimization of their emission should be the goal of any project.

b. **Carbon Mono Oxide**

CO constitutes a lesser volume of combustion products from gas turbines but they are eventually converted to CO₂ hence their emission is controlled for the same reason.

c. **Sulphur Oxides (SOₓ)**

SOₓ and SOₓ which in the presence of moisture are converted to sulphurous acid (H₂SO₃) and sulphuric acid (H₂SO₄), have been directly linked to acid rain, which has been responsible for alteration of certain aquatic ecosystems, damage to vegetation and deterioration of building materials. SO₂ is also particularly detrimental to health, as it is known to aggravate asthma, lung and heart diseases.

d. **Nitrogen Oxides (NOₓ)**

Oxides of nitrogen, in the presence of water form Nitrogen and Nitric acids, contributing to acid rain and are some of the ingredients in photochemical smog. High levels of NOₓ are thought to increase the risk of respiratory diseases and contribute to heart, lung, liver and kidney damage and eye irritation. High NOₓ levels also cause damage to vegetation.
8.0 METIGATION METHODS
Various methods are employed to mitigate the impact of combustion pollutants on either human health or the environment. Some of the control strategies employed in industry include the following:-

- prevention (better design, stringent regulatory enforcement)
- minimization (add-on controls (technological), work practices)

At the Takoradi Thermal Power Plant, a mixture of both prevention and minimization methods are being used to mitigate the overall impact of plant emissions.

The design of the plant incorporated a modeled stack height that improves the eventual dilution and dispersion of the flue gas. This helps to distribute the impact of the emitted pollutant over a wide ground surface area and reduces the average ground level concentration and the impact on vegetation.

As a result of the stringent regulatory requirements by the Ghana EPA and the Project funding agencies, the Environmental Impact Assessment restricts emissions from the plant to one-third of the allowable World Bank ground level concentration guidelines for NOₓ emissions. This restriction was based on the possibility of expansion of the present facility and the fact that other industries of similar nature could be sited in the same area in the future.

For the control of NOₓ emissions, the technology of water injection was also incorporated into the Plant design whereby water is sprayed into the combustion chamber to reduce the combustion temperature and hence minimise the level of NOₓ emitted into the atmosphere.

The concentration of fuel nitrogen content for the light crude oil imported for burning at Takoradi Thermal Power Plant is also limited to 120 mg/I to minimise NOₓ emission.

SO₂ control is achieved by limiting the fuel total sulphur content to 0.2% by weight to ensure that SO₂ emissions fall within acceptable guidelines.

8.1 MONITORING
At the Takoradi Thermal Power Plant, monitoring of emission from the combustion turbine is accomplished by the means of a continuous emissions monitoring system (CEMS) set up for the purpose.

A sample of the exhaust gas is passed through NOₓ, CO₂, CO and SO₂ gas analyzers. The concentration of each gas pollutant in the exhaust system is displayed on the analyzer screen. Both instantaneous and average reading are recorded.

The ambient ground level concentrations of NOₓ & SO₂ are monitored with similar analyzers installed at 3 locations corresponding to:-

- the point of maximum out fall of airborne plant emissions
- the nearest community
- background monitoring station

8.2 NOₓ MONITORING INSTRUMENTATION
The NOₓ analyzer at the Takoradi Thermal Power Plant uses a gas-phase chemiluminescence detection to perform continuous analysis of nitric oxide (NO), total oxides of nitrogen (NOₓ), and nitrogen dioxide (NO₂).
The instrument consists of a pneumatic system, an NO₂-to-NO converter, a reaction cell, a detector (PMT), and processing electronics.

The pneumatic system continuously supplies particulate-free sample air to the measurement cell at a rate that allows the sample to be measured before exiting the analyser. The pump pulls a slight vacuum that causes sample air to be drawn into the sample inlet and through the five-micron particulate filter. The sample then flows through a critical orifice which maintains constant flow and strong vacuum in the reaction cell.

The method is based on the luminescence from an activated molecular NO₂ species produced by the reaction between NO and ozone (O₃) in an evacuated chamber. The NO molecules react with ozone to form the activated species NO₂* according to the reaction mechanism:

\[ \text{NO} + \text{O}_3 = \text{NO}_2^* + \text{O}_2 \]

As the activated species, NO₂*, reverts to a lower energy state, it emits broad-band radiation from 500 to 3000 nm, with a maximum intensity at approximately 1100 nm. Since one NO molecule is required to form one NO₂* molecule, the intensity of the chemiluminescent reaction is directly proportional to the NO concentration in the sample. The detector (PMT) current is then directly proportional to the chemiluminescent intensity.

In order to measure the zero offset of the instrument, a background measurement is performed every 135 seconds by diverting the sample flow from the reaction cell to the cell bypass line. This measurement is electronically subtracted from all subsequent measurements to achieve very stable measurements.

8.3 SO₂ MONITORING INSTRUMENTATION

The sulphur dioxide analyser at TTPP is based on classical fluorescence spectroscopy principles. SO₂ exhibits a strong ultraviolet absorption spectrum between 200 and 240 nm. Absorption of photons at these wavelengths results in the emission of fluorescence photons at wavelengths between approximately 300 and 400 nm. The amount of fluorescence emitted is directly proportional to the SO₂ concentration. These characteristics are exploited by the analyser.

UV radiation at 213.9 nm from a zinc discharge lamp is separated from the other wavelengths in the zinc spectrum by an optical band-pass filter. The 213.9 nm radiation is focused into the fluorescence cell where it interacts with SO₂ molecules in the beam path. The resulting fluorescence is emitted uniformly in all directions. A portion of the fluorescence, i.e. that emitted perpendicular to the excitation beam, is collected and focused onto a photo multiplier tube. A reference detector monitors the emission from the zinc lamp and is used to correct for temporal lamp fluctuations. Figure 8 shows the System Block Diagram.

The pneumatic system continuously supplies particulate-free sample air to the measurement cell at a rate that allows the sample to be measured before exiting the analyser. The pump pulls a slight vacuum that causes sample air to be drawn into the sample inlet and through the five-micron particulate filter. The sample flow then enters the hydrocarbon kicker where possible hydrocarbon interferents are removed. After being scrubbed of hydrocarbons, the sample enters the fluorescence cell where the SO₂ measurement is accomplished.
8.4 CO AND CO\(_2\) MONITORING INSTRUMENTATION

The analysers for measuring CO and CO\(_2\) are a non-dispersive infrared (NDIR) photometer that uses gas filter correlation technology to measure low concentrations of both gases accurately and reliably. Infrared broad band radiation is passed through a rotating gas filter wheel where half of the filter wheel contains either CO or CO\(_2\) and half contains nitrogen. When the IR radiation passes through the nitrogen half of the wheel, all wavelengths at which CO or CO\(_2\) can absorb are completely removed from the radiation, leaving those wavelengths that are not affected by CO or CO\(_2\) to create a reference beam.

When IR radiation passes through the nitrogen half of the wheel, CO or CO\(_2\) specific wavelengths are not removed from the radiation. This creates a measure beam that is attenuated by any CO or CO\(_2\) in the sample. The rotation of the gas filter, in effect, creates a beam that attenuates between reference and measure phases. The alternating beam is passed through a multipass absorption cell, where CO or CO\(_2\) is monitored by measuring the attenuation of the measurement beam. Because both the reference and measure phases of the beam have the same source, detector, and optical path, only the amount of CO or CO\(_2\) in the sample cell can affect the difference in the intensity between the two phases. This method of measurement results an instrument that is very insensitive to interfering gases, fluctuations in the IR source, vibration, and accumulation of dust on the optics.

The final concentration of CO or CO\(_2\) correct for temperature and pressure changes is displayed in ppm or mg/m\(^3\).

9.0 MONITORING RESULTS

The levels of emissions of NO\(_x\) from the Takoradi Thermal Power Plant when water injection (NO\(_x\) control) is in service range between 101 - 115 ng/J. The World Bank guideline limit is 130 ng/J. The World Bank guideline limit is 130 ng/J. The EIA for the Plant predicted 100 ng/J. For SO\(_2\), emissions range between 80 - 202 ng/J. The World Bank guideline is 258 ng/J and the EIA prediction is 93 ng/J. It can be observed that with the water injection fully commissioned and operating, the emissions from the Plant are in compliance with both local and international regulatory requirements. The water injection system is still being commissioned by the contractor. Without water injection, NO\(_x\) and SO\(_2\) emissions could rise to more than twice the above values.

9.1 MAJOR PROBLEMS ENCOUNTERED

The following are two (2) major problems have been encountered at the Takoradi Thermal Power Plant with the gas turbines:

9.1.1 EXHAUST DUCT EXPLOSION

In March, 1998 an explosion occurred in the exhaust duct of Gas Turbine #1 (GT1). The unit had been restarted according to the GE hot restart procedure after a trip caused by transmission system fault. The trip was attributed to inadequate purging and leaking check valves. The re-starting procedure after a trip when firing LCO has been modified.
9.1.2 HOT CORROSION

During an inspection to determine the time for a combustion inspection, holes were found in the transition pieces (TPs). The combustion inspection was therefore performed soon afterwards. Deposits found on the TPs tested as Sodium Sulphate which was attributed to fuel quality. The tank farm management and fuel treatment and testing frequency were therefore changed.

Map of the Volta River Authority's Transmission Network in Ghana (As at the end of 1996)

Fig. 1
Combustion Diagnostics and Optical Techniques 336

300 MW Combined Cycle - Being Implemented

600 MW Ultimate Thermal Power Plant Development at Abroadz - Volta River Authority
Fig. 4
SCHEMATIC DIAGRAM OF COMBINED CYCLE PLANT

TAKORADI THERMAL POWER PROJECT
VOLTA RIVER AUTHORITY

Figure 5
Flame Temperature and Fuel/Air Ratio

Fig 7
COMBUSTION PROCESS AT VALCO
Ebenezer Avotri
Valco, Tema

1.0 Oil Supply

Oil to Valco for our furnaces is from the Tema Oil Refinery (TOR) by road using tankers. The oil is Bunker 'C' Residual Oil, viscosity at 100°F of 74 SSU with a Heat Value of 19,302 BTU/lb. The oil is delivered into two reservoir tanks with a capacity of 500,000 gallons each. The steam jackets in these tanks keep the oil hot to temperatures of 100°F. The oil is now pumped through electrically heat traced pipes into smaller storage steam jacketed tanks at the usage points. Temperatures on these tanks can be adjusted depending on weather conditions.

1.1 The standby oil system is the Diesel fuel. To serve as
i. Standby oil for furnaces
ii. Crude Heating System
iii. To shut down furnaces

2.0 Burners

Valco has seven CHARGING (MELTING) Furnaces and 3 (three) Holding Furnaces. See attached. Scrap/Molten metal are charged into the Melting furnaces and transferred into the Holding furnaces from where it is cast into billets and rolling ingots after attaining appropriate conditions of temperature, chemistry, etc.

2.1 Capabilities of ‘214’ Oil Burners
i. Eliminate Carbon buildup
ii. Reduce routine maintenance
iii. Maintain controlled furnace atmosphere
iv. Operate from very lean to rich mixture (air/oil ratio)
v. Hold positive or negative furnace pressure
vi. Provide stable burning with light or heavy oil

Series 214 Oil Burners are Nozzle-Mix Sealed-in burners for operation on light or heavy oil. These burners are capable of operating with equal proficiency throughout a wide temperature range – from low temperature ovens to high temperature forge and melt furnaces (about 760°C).

3.0 Air Sup.

Valco uses combustion blowers with capacities in the attached.
3.1 Purpose

The purpose of the air supply is to support the combustion system. These are mounted on the mezzanine above each furnace. They supply sufficient volume and pressure to obtain correct combustion with the burners mounted on furnaces. All fans are rated at 24 OSI discharge pressure. The fans run at constant speeds and produce a constant amount of air and no controls are installed to vary their operation. The combustion air is broken into two groups:

- Main air
- Atomizing air

The Main Air leaves the fan and is controlled by actionator motors/valves to the burners to obtain desired pressures and flows.

The Atomizing Air arrives at the burner at a slightly lower than the discharge pressure of the blower (24 OSI) to break the stream of fuel oil into tiny particles for better oil/air mixer resulting in better combustion.

3.6 Burner Safety (Burner Sensor)

The furnace safe operation is maintained by a flame detector by insuring that fuel is being burnt as it flows out of the burner. The flame detector (PC II Scanner-4915) is wired to the control relay for the safety solenoid valve, so if the flame is not detected, the safety solenoid valve closes.
ULTRA-STABLE COMBUSTION
- Plants keep burning even under adverse conditions, allowing burners to:
  - Run with very lean or very rich settings.
  - Maintain constant temperature atmosphere.
  - Operate in cold climate conditions.
  - Pass excess air for reduced temperature uniformity.

UNCONDITIONAL COMBUSTION
- Versa burners operate dependably under a wide variety of conditions, with:
  - Any gas, any oil—changing without disturbing process operation.
  - Positive or negative furnace pressure.
  - Both or lean burn air intake.
  - Wide turndown range.

EASY OPERATION—MINIMUM MAINTENANCE
- The stable, safe, easy ignition.
- Quick combustion termination.
- Observation port, stable flame section.
- No carbon build-up.

Combustion Diagnostics and Optical Techniques
COMBUSTION PROCESSES MONITORING
BY ENVIRONMENTAL PROTECTION AGENCY IN GHANA

Dyson T. Jumppah,
Environmental Protection Agency
Accra, Ghana

ABSTRACT

Air pollution in Ghana has traditionally been associated with industrial activities, domestic wood fuel burning, bush burning and solid wastes burning at 'landfills'dumping sites. The EPA has over the years been monitoring emissions from these sources using active samplers. The monitoring sites include industrials, commercial and residential. In recent years, the consumption of fossil fuels by the transport sector and its associated air emissions have grown significantly to match or exceed other sources of most of the important pollutants. In the urban areas vehicle exhaust emission have become the dominant sources of air pollutants. The EPA has identified and procured the appropriate vehicle exhaust emission diagnosis equipment. Further, the Agency has proposed a collaborative programme for a national monitoring and control of air pollution from motor vehicles. A pilot vehicle exhaust emission testing programme using diagnostic gas analyser was launched recently by the EPA. Prior to, the EPA has developed procedure for vehicle exhaust emission diagnosis.

1.0 INTRODUCTION

Air pollution is a major problem facing all nations of the world. Various chemicals are emitted into the air from both natural and man-made sources. Emissions from natural sources include those from living and non-living sources (e.g. plants, radiological decomposition, bush fires, volcanic eruptions and emissions from land and water). These emissions lead to a natural background concentration that varies according to the local source of emission and the prevailing weather conditions. People have caused air pollution since they learned how to use fire, but man-made air pollution (anthropogenic air pollution) has rapidly increased since industrialisation began.

Research over the past two decades has revealed that in addition to the previously known common air pollutants (sulphur oxides, nitrogen oxides, particulate matter, hydrocarbons and carbon monoxide) many volatile organic compounds and trace metals are emitted into the atmosphere by human activities. Although our knowledge of the nature, quantity, physico-chemical behaviour and effects of air pollutants has greatly increased in recent years, more needs to be known about the fate and transformation of different pollutants and about their combined (synergistic) effects on human health and the Environment.
2.0 COMBUSTION PROCESSES

Combustion is the most widely used, and yet one of the least understood, chemical reactions at our disposal. Combustion is defined as the rapid union of a substance with oxygen accompanied by the evolution of light and heat (1).

We use combustion primarily for heat by changing the potential chemical energy of the fuel to thermal energy. We do this in a fossil fuel-fired power plant, a furnace or an automobile engine. We also use combustion as a means of destruction for our unwanted materials. We reduce the volume of solid waste by burning the combustible in an incinerator or at a "landfill". We subject combustible gases, with undesirable properties such as odour, to high temperature in an after burner system to convert them to less objectionable gases.

The simple combustion equations are very familiar:

\[
\begin{align*}
C + O_2 & = CO_2 \\
2H_2 + O_2 & = 2H_2O
\end{align*}
\]

The combustion products are carbon dioxide and water, under ideal conditions which are odourless and invisible.

The problems with the combustion reaction occur because the process also produces many other products under real conditions most of which are termed air pollutants. These can be carbon monoxide, carbon dioxide, oxides of sulphur, oxides of nitrogen, smoke, fly ash, metal oxides, metal salts, aldehydes, ketones, acids, polynuclear hydrocarbons, and many others. Only in the past few decades have combustion engineers become concerned about these relatively small quantities of materials emitted from the combustion process. An automotive engineer for example was not overly concerned about the 1% of carbon monoxide in the exhaust of the gasoline engine. By getting this 1% to burn to carbon dioxide inside the combustion chamber, the engineer could expect an increase in gasoline mileage of something less than one-half of 1%. This 1% of carbon monoxide, however, is 10,000 ppm by volume, and a number of such magnitude cannot be ignored by an engineer dealing with air pollution problems.

Combustion is extremely complicated but is generally considered to be a free radical chain reaction. Several radical mechanisms including the following occur:

(i) Simple calculations of the heats of dissipation and formation for the molecules involved do not agree with the experimental values obtained for heats of combustion.

(ii) A great variety of end products may be found in the exhaust from a combustion reaction. Many complicated organic molecules have been identified in the effluent from a system burning pure methane with pure oxygen.

(iii) Inhibitors, such as tetraethyl lead, can greatly change the rate of reaction.

When visualizing a combustion process, it is useful to think of it in terms of the three Ts: time, temperature and turbulence. Time for combustion to occur is necessary. A combustion process that is just initiated, and suddenly has its reactants discharged to a chilled environment, will not go to completion and will emit excessive pollutants. A high enough temperature must
exist for the combustion reaction to be initiated. Combustion is an exothermic reaction (it gives off heat), but it also requires energy to be initiated.

Turbulence is necessary to ensure that the reacting fuel and oxygen molecule in the combustion process are in intimate contact at the proper instant, when the temperature is high enough to cause the reaction to begin. The physical state of the fuel for a combustion process dictates the type of system to be used for burning. A fuel may be composed of volatile material, fixed carbon or both. The volatile material burns as a gas and exhibits a visible flame whereas the fixed carbon burns without a visible flame in a solid form. If a fuel is in the gaseous state, such as natural gas, it is very reactive and can be fired with a simple burner.

If a fuel is in the liquid state, such as fuel oil, most of it must be vaporised to the gaseous state before combustion occurs. This vaporisation can be accomplished by supplying heat from an outside source, but usually the liquid fuel is first atomised and then the finely divided fuel particles are sprayed into the hot combustion chamber to accomplish the gasification.

With a solid fuel, such as coal or wood, a series of steps are involved in combustion. These steps occur in a definite order, and the combustion device must be designed with these steps in mind.

The cycle of operation of the combustion source is very important as far as emissions are concerned. A steady process, such as large steam boiler, operates with a fairly uniform load and continuous fuel flow. The effluent gases, along with any air pollutants, are discharged steadily and continually from the stack. An automobile on the other hand is a series of intermittent sources. The emissions from the automotive engine will be vastly different from those from the boiler in terms of both quantity and quality. A four-cylinder automotive engine operating at 2500rpm has 5000 separate combustion processes started and completed each minute of its operation. Each of these lasts about 1/100 second from beginning to end.

The emission from combustion processes may be predicted to some extent if the variables of the processes are completely defined. A comparison of typical emissions from various common combustion sources may be seen in table 1.
TABLE 1

<table>
<thead>
<tr>
<th>Pollutant</th>
<th>Power plant emission (gm/kg fuel)</th>
<th>Refuse burning emission (gm/kg refuse)</th>
<th>Uncontrolled automotive emission (gm/kg fuel)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Oil</td>
<td>Gas</td>
<td>Opening burning</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>Nil</td>
<td>Nil</td>
<td>Nil</td>
</tr>
<tr>
<td>Oxides of Sulphur (SO₂)</td>
<td>(20)x</td>
<td>(16)</td>
<td>1.5</td>
</tr>
<tr>
<td>Oxides of nitrogen (NO₂)</td>
<td>0.68</td>
<td>0.16</td>
<td>2.0</td>
</tr>
<tr>
<td>Aldehydes &amp; Ketones</td>
<td>0.003</td>
<td>0.001</td>
<td>3.0</td>
</tr>
<tr>
<td>Total hydrocarbons</td>
<td>0.05</td>
<td>0.005</td>
<td>7.5</td>
</tr>
<tr>
<td>Total particulate</td>
<td>2.8y</td>
<td>Nil</td>
<td>11</td>
</tr>
</tbody>
</table>

X = percentage of sulphur in fuel; Y = percentage of ash in fuel.  Source (2)

2.1 Industry/Stationary Sources

Air pollution associated with Ghana’s industrialisation activities result mainly from combustion processes such as the firing of boilers, thermal plants, furnaces, etc. The pollutants from these sources tend to be in varying quantities in the form of particulate matter, smoke, Sulphur dioxide, Carbon dioxide, Carbon monoxide, hydrocarbons etc.

2.2 Transport/Mobile Sources

A mobile source of air pollution can be defined as one capable of moving from one place to another under its own power. According to this definition, an automobile is a mobile source. Generally, mobile source imply transportation, but sources such as construction equipment, gasoline-powered lawn mowers, and gasoline powered tools are included in this category.

Mobile sources therefore consist of many different types of vehicles, powered by engines using different cycles, fuelled by a variety of products, and emitting varying amounts of both simple and complex pollutants.

The predominant mobile air pollution source in all industrialised and developing countries of the world is the automobile, powered by four-stroke cycle (Otto Cycle) engine and using gasoline as the fuel.

Plate 2 shows how air-borne pollutants are emitted from the vehicle into the atmosphere. A significant proportion of the hydrocarbons comes from the fuel tanks and carburettor and the crank-case, but the exhaust gases are the major source of pollutants.
If combustion is complete in the engine, water and carbon dioxide would be the only products of the combustion fuel. Some years ago, it would have been possible to assert that neither of these is a pollutant, however although we can still assume that this is true about the water, it cannot be taken for granted about carbon dioxide.

In practice complete combustion is impossible to achieve, and carbon monoxide is formed in considerable quantities. Some fuel is emitted unchanged, and some is converted into other organic compounds. Apart from these products of incomplete combustion many petrol contain “anti-knock” agents that contain lead, and lead compounds are therefore found in the vehicle exhaust. Sulphur dioxide in the atmosphere is primarily the product of power stations and other industrial processes and is not an important aspect of road pollution, but in densely trafficked areas the concentrations emitted by vehicles, mainly diesels, may require consideration. In addition the conditions in the combustion chamber favour the oxidation of the nitrogen in the air so that oxides of nitrogen are also formed. The compounds present in the exhaust gases are:

**Water vapour (H₂O):** Not considered to be a pollutant. It is formed during combustion when hydrogen from the fuel and oxygen from the air combine. H₂O is a product of complete combustion. The more fuel burned the more water produced.

**Carbon dioxide (CO₂):** is not previously considered as a pollutant. It is formed during combustion when carbon from the fuel and oxygen from the air combine. CO₂ is a product of complete combustion. The more fuel burned the more CO₂ produced. Insufficient oxygen results in less CO₂.

**Carbon monoxide, CO** is formed during combustion when carbon from the fuel and oxygen from the air combine. CO is a product of incomplete combustion. Insufficient oxygen will produce higher quantities of CO. Road vehicles account for some 85% of total CO emissions in the UK and most of this comes from petrol engine vehicle (3).

**Hydrocarbons HC** in the same form as it entered the engine. HC’s in the exhaust are due to incomplete combustion. The better the combustion less HC will be present.

**Oxides of Nitrogen** are formed due to high combustion temperatures. Very weak mixtures will cause an increase in temperature and therefore more NOₓ. Road traffic is responsible for 51% of NOₓ emissions (3).

Other components of vehicle exhaust gases are, sulphur dioxide, Carbon particles (smoke) Lead compounds etc.

The smoke listed is produced in the form of very fine particles of carbon also resulting from incomplete combustion, which acts as a nucleus (see fig. 4) for other materials, usually in diesel engines. This smoke is the only item that is always clearly visible and for that reason gives rise so much comments from the public.
3.0 ENVIRONMENTAL IMPACTS OF COMBUSTION

The harmful effects of air pollutants on human beings and the environment have been the major reason for efforts to understand and control their sources.

Many air contaminants are emitted by industry. The quantities and types of compounds emitted depend on many factors in particular the type of industry, the characteristics and quantities of raw material used, the type and quality of fuel, the technology applied, and the environmental protection measures in place. Factors such as the size of the industrial installation, the age of the machinery, and the standard of maintenance and management are important. In addition to the common emissions into the air, such as sulphur and nitrogen oxides, carbon dioxide, carbon monoxide, hydrocarbons and particulate matter, industry emits hundreds of trace contaminants, some of which are potentially toxic.

World-wide, 99 million tonnes of sulphur oxides ($\text{SO}_x$), 68 million tonnes of nitrogen oxides ($\text{NO}_x$), 57 million tonnes of suspended particulate matter (SPM) and 177 million tonnes of carbon monoxide (CO) were released into the atmosphere in 1990 as a result of human activities, from stationary and mobile sources. The Organisation for Economic Co-operation and Development (OECD) countries accounted for about 40% of the $\text{SO}_x$, about 52 per cent of the CO, and for 23 per cent of the SPM emitted into the global atmosphere, the rest of the world accounted for the remainder (4).

At very high levels, prolonged exposure to carbon monoxide can result in death. At lower levels, the reduction in the oxygen-carrying capacity of the blood may increase the risk of heart problems in predisposed individuals.

The main source of carbon monoxide in Ghana is road transport. Of this road transport emission, the predominant source is petrol vehicles. The estimates of the metric tonnes of emissions from the transport sector are not yet available. This needs to be done so that the proportional contributions from the various combustion processes could be determined, impacts adequately predicted and addressed.

Emission of CO may also be important climate modification. The reason for this is that highly reactive hydroxyl radical (OH) which scavenge many anthropogenic and natural trace gases from the atmosphere are themselves used in the oxidation of CO. Thus the increase in CO that is taking place can increase the concentration of several other greenhouse gases such as ozone ($\text{O}_3$), methane ($\text{CH}_4$) and NO.

$\text{CO}_2$ emitted by vehicles causes global warming (green house effect). A single tank of petrol produces more than 100kg of $\text{CO}_2$ when burned; motor vehicles provide more than 15% of the world’s total $\text{CO}_2$ emission and these are set to increase rather than decrease, while CO2 produced by individual processes is that CO2 is actually a product of good combustion, not bad. The only method available to reduce these emissions therefore is to burn less fuel oil, which means either fewer vehicles, or vehicles more economical with fuel, or totally different power sources, or some combination of these.

Exposure to nitrogen dioxide can bring about reversible effects on lung function and airway responsiveness. It may also increase reactivity to natural allergens. Exposure to nitrogen dioxide may put children at increased risk of respiratory infection and may lead to poorer lung function in later life.
The main precursors of acid deposition are sulphur dioxide (SO$_2$) and nitrogen oxides (NO$_x$) emitted into the atmosphere from combustion processes. Exhaust emissions from motor vehicles contribute most of the NO$_x$ whilst the Sox comes mainly from the power stations and other fuel burning installations. Hydrocarbon emitted into the atmosphere can in the presence of oxides of nitrogen, take part in photochemical reactions yielding a range of noxious species including ozone, NO$_2$, aldehydes, peroxyacetyl nitrate (PAN) and aerosol species. Thus although hydrocarbon themselves do not contribute to acid deposition they are involved in the production of species that do.

Most of the air borne emissions of lead arises from petrol engine motor vehicles. This is a prevalent situation in Ghana since only leaded fuel is available in the country. Lead exhibits toxic biochemical effects in humans, which are manifest in the synthesis of haemoglobin, acute or chronic damage to the nervous system, effects on kidneys, gastrointestinal tract, joints and reproductive system.

Unlike the individual gaseous pollutants which are single, well-defined substances, particulate matter in the atmosphere is composed of a wide range of materials arising from a variety of sources. Examples of man-made sources are: carbon particles from incomplete combustion; ash; recondensed metallic vapours; and so-called secondary particles, or aerosols, formed by chemical reactions in the atmosphere. As well as being emitted directly from combustion processes, man-made particles can arise from: mining, quarrying and construction operations; brake and tyre wear in motor vehicle; and from road dust resuspended by moving traffic or strong winds. Particulate air pollution appears to be associated with a range of measures of ill-health including effects on: the respiratory and cardiovascular systems, asthma, and mortality.

4.0 MONITORING OF COMBUSTION PROCESSES BY EPA

4.1 Monitoring Objective
Monitoring of air pollution in Ghana began since the late 1970’s by the erstwhile EPC. The fundamental objective of the monitoring programme was to provide adequate assessment of the ambient air pollutant (particulates) the EPC has the capacity to monitor in order to prepare Air Quality Guidelines. These Guidelines are to be converted into National Air Quality Standards.

Road vehicle population has increased significantly over the past decade with the attendant increase in vehicular emissions. The emission of exhaust pollutants such as carbon monoxide, carbon dioxide, oxides of nitrogen, hydrocarbons and smoke have negative impacts on public health and the environment. In this regard the EPA identified under Ghana Environmental Resources Management Project (GERMP) the need for capacity development in the areas of Vehicle exhaust testing/monitoring technology, vehicle exhaust emission guidelines, standards setting, awareness creation and compliance enforcement procedures. These requirements are considered critical for air pollution control from motor vehicles.

For the EPA, the essence of the vehicle exhaust emission control is to:

(i) Help keep our air clean and protect public health;
(ii) Reduce the emission of smoke, carbon monoxide, hydrocarbons, and oxides of nitrogen so as to eliminate or minimise the nuisance to road users and
(iii) Ensure that vehicles run efficiently to reduce cost to the vehicle owner in terms of fuel consumption, performance and reliability.

4.2 Monitoring Methodology

Air quality monitoring involves measuring the actual ambient concentration of pollutants in air at given place and point in time. The measurement produced is always an average value over a defined period of time, which may range from a month to a few seconds. A variety of techniques of varying sophistication exist for measuring concentration of pollutants in air. The methods fall into four main groups:

- Passive sampling (e.g. diffusion tube)
- Active sampling (bubblers, filters etc)
- Automatic point monitoring
- Long path/remote monitoring

4.2.1 Industry Sources

Presently, the EPA employs the active samplers (bubblers, filters) and high volume samplers for the monitoring of air pollutants, particularly SO$_2$, smoke and PM10 from sources such as factories, power plants, construction works, fuel combustion, open burning, quarrying and surface mining operations.

Black Smoke

The equipment being used is the SO$_2$-Smoke Bubbler. The principle of the method involves drawing air at a controlled flow rate through a filter. Suspended particulate matter is collected on the filter, forming a dark stain. The darkness of the stain is measured using a reflectometer, and the reflectometer measurement is used to calculate the concentration of particulate matter in the sampled air.

The term "black smoke refers" to any fine dark suspended particulate which can be measured by this smoke technique, not necessarily particulate resulting from combustion sources. Black smoke is defined in the ISO Standard 9834 as "strongly light absorbing particulate material suspended in the ambient atmosphere...The major contributor to black smoke is soot particles; i.e. particles containing carbon in its elemental form". Such particles remain suspended in the air as they are too small to fall under their own weight. In this important respect, the black smoke method differs from deposit gauge techniques which measures deposited particulate.

Sulphur Dioxide (SO$_2$)

The equipment being used is the SO$_2$-Smoke Bubbler. The concentration of SO$_2$ in the air is estimated by passing the same measured samples of filtered air through a dilute solution of hydrogen peroxide in Drehsel bottle (bubbler). Sulphur dioxide in the sampled air reacts with the hydrogen peroxide to form sulphuric acid solution. The amount of acid is determined by titration with a standard alkaline solution. Other strong alkalis or acids in the air will affect the result, so technically this method measures total acidity rather than SO$_2$. However, in normal circumstances
the concentration of such substances is very much less than that of SO₂. Therefore the result obtained is usually a good approximation to the concentration of sulphur dioxide.

The dilute hydrogen peroxide is acidified to pH 4.5 before use in the bubbler. This ensures that predominantly strong acids are absorbed, rather than weakly acidic compounds such as carbon dioxide. After exposure, the solution is titrated back to the pH 4.5 end point.

PM10
PM-10 Size Selective Hi Volume Air Samplers is the equipment used for PM10 monitoring. Suspended particulates in the air are sampled at 40 cubic feet per minute (CFM) through the circumferential inlet of the size selective inlet. The symmetrical design ensures wind-direction insensitivity, and the inlet design and internal configuration makes the collection efficiency independent of wind speed from 0 to 24 kilometers per hour. The particles are then accelerated through multiple circular impactor nozzles. By virtue of their large momentum, particles greater than the 10microns impactor cut point impact onto the greased impaction surface. The PM10 particles smaller than 10microns are carried vertically upward by the air flow and down multiple vent tubes to an 8-inch x 10 inch hi-vol filter, where they are collected. The larger particles settle out in the impaction chamber on the collection plate and are removed/cleaned during maintenance periods. The hi-vol filter is weighed before and after sampling. The weight increase is the mass of smaller 10microns. The mass concentration of PM10 particles (microns per cubic meter) by the sampled air volume (cubic meters). The volume is properly totalled by maintaining a constant flowrate of 40CFM (68 cubic meters per hour).

4.2.2 Road Transport
The monitoring of air pollution from motor vehicles is an absolutely new programme being initiated by the EPA. For this reason the EPA was plagued with the problem of identifying and acquiring the modern scientific equipment for motor vehicle emission testing/monitoring. Under the Ghana Environmental Resources Management Project (GERMP), the EPA through a collaborative programme with the Hackney Environmental Council and Vehicle Inspectorate Department of the United Kingdom has acquired the technology of vehicle exhaust emission testing/monitoring.

Petrol Engine Vehicles Emission Testing
The Diagnostic Gas Analyser (DGA-1800) is a compact unit designed for garage use. It is equipped with a four (4) Gas Bench, a 14" colour Monitor, a printer and a Keyboard. It has an inbuilt Software structured using simple menus which lead the operator through a general purpose programme of measurement modes and limited vehicle diagnostics. The Diagnostic Gas Analyser 1800 is the vehicle exhaust analyser the EPA has acquired for the monitoring of vehicle exhaust emissions. This equipment is equipped with a positive ignition (petrol) engine emission sampling and analysis. The Standard unit measures and displays Carbon monoxide (CO), Carbon dioxide (CO₂), Hydrocarbon (HC) content in the exhaust emission of Spark ignition engines by non dispersive infra-red technology and the percentage Oxygen (O₂) content by a galvanic cell.

The Diagnostics capability of the equipment includes the measurement of Lambda and Air Fuel Ratio with high accuracy as well as the comparison of measured values against limits.
Diesel Engine Vehicles Emission Testing

The component of exhaust emission from diesel engine vehicles of concern is Black smoke. The Free Acceleration Smoke Test is the method of obtaining black smoke emissions from a vehicle under test. In this test the vehicle’s engine is run until normal operation temperature is achieved. Then the accelerator pedal is pressed down to its maximum extent and kept there until the engine reaches its governed speed. By this action the engine is accelerated at the maximum possible rate against its own inertia and hence operating at full power (and fuel delivery) through its operating range. The peak smoke level is then detected and recorded. This is repeated several times in order to obtain a mean reading of peak smoke level.

The smoke meter (ASA 200T) uses a modulated light diode (LED) as a light source and a solid state photodiode light receiver and is control by computer within the handset. The computer measures the light level received at the photodiode when attenuated by the exhaust smoke passing through the meter, calculates the density of smoke and records the peak level seen.

The smoke is sampled by a sensor unit inserted into the vehicle exhaust, linked, via a cable that carries power and data to the handset. The sensor unit contains the light source and receiver, a fan for providing a curtain of clean air across the optics and clamp for fixing the unit to the exhaust tail pipe. The handset can be disconnected from the sensor and plugged into its base station which provides charging and link to the printer for output of results. Verification filters are also provided to enable calibration of the meter to be carried out at zero (K=0) and mid point value of approximately K=1.7.

The operation of the meter is controlled by an in-built computer that displays commands and options on the handset display screen. A zero check is performed at the beginning and end of each test to ensure that the optics are not excessively dirty and to enable a correction to be made if not absolutely clean. When the test is started the handset issues commands from the display to start accelerating, to release the throttle and when to start and stop the engine.

5.0 Monitoring Outputs

5.1 Industry

The former Environmental Protection Council with the assistance of World Health Organisation (WHO), the Environmental Protection Authority (Victoria, Australia) and the erstwhile Atomic Energy Authority (AEA) of United Kingdom gathered data on background information on Ghana’s Air Quality for a considerable period. This has enabled the Agency to develop a National Air Quality Guideline. Currently, EPA has some air-monitoring stations at residential, commercial and industrial areas in the country.

5.1.1 Pollutants Monitored

Air pollutants monitored by EPA and presented in this report include SO2, PM10 and Smoke.
5.1.2 MONITORING STATIONS
As at 1998 there were five (5) active monitoring sites (5).

<table>
<thead>
<tr>
<th>Site</th>
<th>Location</th>
<th>Pollutants Monitored</th>
<th>Designation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. West, Coast</td>
<td>Tema heavy industrial area opposite TOR</td>
<td>PM$_{10}$, Smoke, SO$_2$, Smoke</td>
<td>Industrial</td>
</tr>
<tr>
<td>Industries Ltd</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2. Tema General</td>
<td>Tema General Hospital</td>
<td>PM$_{10}$, SO$_2$, Smoke</td>
<td>Residential</td>
</tr>
<tr>
<td>Hospital</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3. G.W.S.C, Accra</td>
<td>Tudu adjacent to the Central</td>
<td>PM$_{10}$, SO$_2$, Smoke</td>
<td>Commercial</td>
</tr>
<tr>
<td>Gov't Hospital</td>
<td>Police Station.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4. Tarkwa Government</td>
<td>Tarkwa Government Hospital</td>
<td>PM$_{10}$, SO$_2$</td>
<td>Mining</td>
</tr>
<tr>
<td>Hospital</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5. EPA, Accra.</td>
<td>EPA, Headquarters building</td>
<td>SO$_2$</td>
<td>Demonstration Station</td>
</tr>
</tbody>
</table>

5.1.3 RESPIRABLE DUST (PM$_{10}$)
This pollutant most noticeable by the public and has its components as dust, soot, smoke, airborne chemicals as solids or liquid droplets or fumes or pollens carried by wind current.

Sampling and measurements is by gravimetric method using the Hi Volume Sampler (PM$_{10}$) over 24 hours averaging time. Fig 1.0 is a plot of the monthly means of PM$_{10}$ concentrations for the 1998-monitoring year at four of the five sites monitored.

Key: Ind = Industrial zone, Res = residential zone, Com = commercial zone, min = mining zone, AM = annual mean, EPAG = EPA guideline value.

No PM$_{10}$ was monitored for the demonstration station because the necessary environmental conditions for siting a Hi volume sampler (such as a sampler being shaded by trees, tall buildings and other sinks) were not met. Besides the mining zone, monitoring was not done at the other zones for March 1998 because of the nation-wide power curtailment during the power crisis.

Fig 1.0: Monthly and Annual mean of PM$_{10}$ monitored for 1998.
From the results, January, February and December are the most polluted months for all the zones. The entire commercial zone is the most polluted followed by the mining, industrial and lastly, the residential zone. Since mining is considered an industrial activity and the PM₁₀ impact at Tarkwa measured in the residential area, it would be appropriate to apply the residential standard to this site until a standard is set for the mining zone.

In this regard, 76μg/m³ has been applied as the standard for the mining zone and the data showed 37.8% exceedance whilst January, February, March and December being the most polluted months. This could be attributed to re-entrained dust from the harrattan winds, enhanced mining activities at Teberebe Goldmines, Ghana Manganese Company at Nsuta, Damang Goldfields Ltd at Aboso, Ghana Australian Goldfield Ltd, Goldfields Ghana Ltd, Bogoso Goldfields Ltd around or reduced rainfall, increased domestic fuel burning, construction or road repair works as well as vehicular emissions. In December 1997, when no mining operations were ongoing, the mean PM₁₀ value recorded was 76.23μg/m³ indicating that most of the values above 76.23μg/m³ during the normal monitoring period could be attributed to surface mining activities.

There was 82% exceedence in the commercial zone, 0% exceedence for residential and 2% exceedence for the industrial zone of which 5 days were due to the fire disaster at Tema Oil Refinery (TOR).

5.1.4 SULPHUR DIOXIDE (SO₂)

The SO₂ bubbler was used for sampling both SO₂ and smoke over 24-hour averaging time. The bubbler has 8 ports. Ambient SO₂ is drawn into drescher bottles containing acidified hydrogen peroxide to form dilute H₂SO₄. This is then titrated against standard borax solution to obtain the SO₂ concentration.

The data presented are for 4 out of the 5 sites. Fig 2.0 represents monitored at 4 sites for 1998

The annual means (in μg/m³) of SO₂ for 1997 representing industrial, residential and
commercial zones were 26.7, 35.4 and 7.8 respectively. The highest value registered then was 50.80 μgm\(^{-3}\) in October (as against 55.10 μgm\(^{-3}\) in the residential area but for January in 1998). In 1998, the annual means recorded are 11.86, 18.93, 9.12 and 13.15 μgm\(^{-3}\) representing residential, industrial, commercial, and the Demonstration Station (DS) respectively with the highest value as 64.97 μgm\(^{-3}\) in the industrial zone.

For 1997, the residential area was more polluted than the industrial area in terms of SO\(_2\), the data for 1998 shown in fig 2.0 however indicates the industrial zone as most polluted. The graph further indicates that the stations area of Accra (mean as 13.15 μgm\(^{-3}\)) is relatively more polluted than the residential area (11.86 μgm\(^{-3}\)).

5.1.5 SMOKE

The same 8-port SO\(_2\) bubble used to monitor SO\(_2\), measures the level of smoke over 24-averaging time. Filters are placed in clamps to filter the air drawn in by the motor before entering the drencher bottles. All particulates are removed from the air as smoke. The reflectance of the sampled filter papers are then determined using a reflectometer and matched against ISO standard chart for the smoke concentration (μgm\(^{-3}\)). Fig 3.0 shows the monthly mean of smoke monitored for 1998.

In 1997, the annual smoke means were 11.6, 7.0 and 89.4 representing the industrial, residential and commercial zones respectively indicating the commercial zone as the most polluted. For 1998, the annual means of 19.64, 16.92, 132.39 and 35.39 representing industrial, residential, commercial and the DS respectively indicate 1998 as more polluted than 1997. The highest value recorded for 1998 is 760 μgm\(^{-3}\) in January for the commercial zone. The conditions at the DS are close to that of the commercial site and hence most of the smoke could be due to vehicular emissions and open incineration of solid waste. The industrial area recorded its highest value as 100 μgm\(^{-3}\) on the day TOR had a fire disaster.

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5.2 Road Transport

In collaboration with the Hackney Environmental Division of the United Kingdom and the Vehicle Inspectorate Department of United Kingdom, the EPA has selected internationally approved scientific exhaust emission analysers for use in Ghana. Further, the Agency has undertaken the following concrete actions for the commencement of pilot exhaust emission testing:

(i) Acquired one petrol engine vehicle exhaust emission analyser and two (2) diesel engine vehicle exhaust analysers;
(ii) Trained four senior officers on the use of the analysers; i.e. two from VELD and two from MTTU and
(iii) Developed a procedure for the vehicle exhaust emission testing.

Consistent with the strategy that environmental management is best done in a collaborative fashion, the EPA, VELD and MTTU are working together to conduct the pilot exhaust emission testing to aid the development of emission guidelines/standards.
After the initial trial period, vehicles would be expected to conform to the guidelines. The EPA will continue to give technical assistance to VELD and MTTU to ensure the compliance and enforcement of the standards that will be set. We will continue to collaborate with VELD and MTTU to carry out this exercise to ensure the maintenance of good air quality in the country.

5.2.1 Vehicle Exhaust Emission Testing Procedures
5.2.1.1 Petrol Engined Vehicles

(i) Checks on the Vehicle before the Test
As a general precaution motorists or testing officers are advised to check that the vehicle has enough engine oil, the coolant level is correct, topped-up, and there is enough fuel to carry out the test. If defects are known before the test then it is advisable to have these rectified well in advance of the test appointment. Wherever possible vehicles should arrive at the test station with the engine at its normal operating temperature (e.g. after a drive of around 5 miles).

Before carrying out the test, the tester will confirm that the engine is at its normal operating temperature which, in some cases will require the use of a temperature probe inserted into the dipstick tube. Before proceeding the tester will also check that the engine has adequate oil and fuel to complete the test.

For vehicles with manual transmission the test be carried out with the gear lever in the neutral position and with the clutch engaged. For vehicles with automatic transmission the gear selector will be in the either the neutral or parking position.

(ii) Visual Inspection
Once the preliminary checks have been completed, the tester will raise the engine speed to around 2500rpm or half the maximum engine speed if this is lower. The engine speed will be held steady for about 20 seconds then the engine will be allowed to return to its natural idle speed. Once the emissions have stabilised the tester will assess the smoke emitted from the tailpipe. If the exhaust is emitting dense blue or clearly visible black smoke then the vehicle will fail the test.

After completing the visual test use the analyser (DGA 1800) to assess the concentration composition of the exhaust gases by inserting a sample probe into the exhaust tailpipe. The test is carried with the engine at its normal idling speed and the analyser displays the results continuously. Once a stabilised figure is achieved the tester will record the result.

(iii) Exhaust Emission Diagnosis
a) Vehicles applying for road user fee or vehicles authorised by MTTU officer for excessive smoke should be directed to VELD testing Site.
b) Testing procedure explained to driver/vehicle owner and vehicle data collected.
c) Result printed, Top Copy given to Driver and explained. The other copy for study by EPA/VELD.
d) Vehicle passes – No Further Action Taken. Vehicle fails, testing officer asks driver for name and address of owner, then serves rectification notice by handing it over to the driver.
e) Vehicle allowed to leave test site and issued the relevant permit needed by VELD
### Vehicle Data Collection Format

**Date:**  
**Time:**  
**Venue:**

<table>
<thead>
<tr>
<th>Registration Number</th>
<th>Petrol/Diesel</th>
<th>Make/Model</th>
<th>Pass/Fail</th>
<th>Possible Problem/Cause</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

(iv) **RANGE OF TYPICAL VEHICLE EXHAUST EMISSION VALUES (3)**  
(Petrol Engine in good condition)

<table>
<thead>
<tr>
<th>EXHAUST GASES</th>
<th>LIMITS</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO % Vol.</td>
<td>1.5% or less</td>
</tr>
<tr>
<td>HC PPM</td>
<td>250 or More (1200)</td>
</tr>
<tr>
<td>CO2 % Vol.</td>
<td>13% or More.</td>
</tr>
<tr>
<td>O2 % Vol.</td>
<td>0.5% - 2%</td>
</tr>
<tr>
<td>Lambda λ</td>
<td>0.9 - 1.10</td>
</tr>
</tbody>
</table>

(v) **Interpretation Of Results Using Lamda (λ) as a Diagnostic Aid (4)**

\[
\begin{align*}
\lambda &= \text{High} \\
\text{CO} &= \text{Low} \\
\text{HC} &= \text{Low} \\
\text{CO}_2 &= \text{Low} \\
\text{O}_2 &= \text{High} \\
\text{CO} &= \text{High} \\
\text{HC} &= \text{High} \\
\text{CO}_2 &= \text{Low} \\
\text{O}_2 &= \text{Low} \\
\end{align*}
\]

= Exhaust Leak

\[
\begin{align*}
\lambda &= \text{Low} \\
\text{CO} &= \text{High} \\
\text{HC} &= \text{High} \\
\text{CO}_2 &= \text{Low} \\
\text{O}_2 &= \text{Low} \\
\end{align*}
\]

= Rich Mixture
5.2.1.3 Diesel Engine Vehicles

(i) **Checks On the Vehicle before the Test**

Same as 5.2.1.2 i

(ii) **Metered Smoke Test**

A metered smoke test using ASA 200T analyser will be carried out for diesel vehicles. Before checking the smoke emission the testing officer will first ensure that the engine speed governor is functioning by increasing the engine speed to about 2500 rpm or half the maximum engine speed steady for 20 seconds then the engine speed will slowly increase to check the operation of the fuel pump governor. Where the engine speed stabilises at its maximum speed, indicating that the governor is working, the engine will then be returned to idle speed. Where it is clear that the governor is not working the engine should be returned to idle speed and stopped, the smoke test will not be carried out – and the testing officer will be unable to pass the vehicle.

Provided the preliminary checks are completed satisfactorily, the tester will next prepare the meter and insert the sampling probe into the exhaust pipe.

Having re-started the engine the tester will start the smoke test. The smoke meter will indicate to the tester where to accelerate the engine and after 2 seconds have elapsed it will display a message telling the tester to release the throttle. The meter will calculate the maximum smoke emission during the acceleration and display the value. A further two accelerations will be requested by the meter. Provided the average of the 3 tests is on or below the appropriate limit in the Table 2, and the three results are within a certain tolerance of each other, then the vehicle will have passed the test. The tester will stop the engine and remove the smoke meter probe from the tailpipe.

Where the average smoke emission at the end of the third acceleration exceeds the limit in Table 1 then the meter will request further tests until either the average of the three preceding accelerations is on or below the limit in the Table or a maximum of six accelerations have been completed. In either case the tester will stop the test and remove the probe from the exhaust tailpipe.

As a final check the tester will assess visually whether the smoke emitted from the exhaust, regardless of measured smoke density is likely to obscure the vision of other road users. If it is likely to do so, in the tester's opinion, then the vehicle will fail the test.

For vehicles with manual transmission the test be carried out with the gear lever in the neutral position and with the clutch engaged. For vehicles with automatic transmission the gear selector will be in the either the neutral or parking position.
Table 1.0  ALL DIESEL FUELED VEHICLES (5)

<table>
<thead>
<tr>
<th>LIMIT</th>
<th>Maximum smoke value (absorption co-efficient) Measured under free acceleration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vehicle Type</td>
<td>Turbocharged Engines</td>
</tr>
<tr>
<td>Passenger cars and light commercial vehicles (&lt;3500kg)</td>
<td>Visual assessment</td>
</tr>
<tr>
<td>All other Vehicles</td>
<td>3.0 per meter</td>
</tr>
</tbody>
</table>

6.0  EVALUATION AND WAY FORWARD

The Agency monitored the air quality for SO₂ and dust particles at these sites for 12 months in 1997. Results of the monitoring were verified by the Quality Control and Quality Assurance Divisions of the National Environmental Technology Centre (NETCEN) of United Kingdom as accurate. These air quality monitoring activities have become an integral part of EPA's work.

In the near future, the Agency will start extensive monitoring of oxides of Nitrogen (NOₓ). Generally, the air quality results so far obtained indicate that the quality of air in our cities and rural areas is quite good, except during the Harnattan season when dust levels are rather high for obvious reasons. On the basis of these findings the EPA is currently working to transform the guidelines into Ambient Air Quality Standards.

The mandated institution to conduct vehicle exhaust emission testing is the Vehicle Examination and Licensing Division (VELD). The EPA is therefore working in partnership with VELD to execute the Vehicle Exhaust Emission Control Programme.

VELD of late has been going through some legislative reviews to enhance their role. This and other institutional arrangements are holding back the Vehicle Exhaust Emission Control (VEEC) programme. However, it is anticipated that as soon as these issues are settled the programme will take off.

The EPA strongly believes in partnership, which fortunately is the major objective of this very important international workshop. We would therefore welcome participants, the universities and other research institutions who would collaborate with the EPA in the following areas among others:

- Application of laser techniques in our National Air Quality Monitoring.
- National pilot motor vehicle exhaust emission testing/monitoring and Vehicle Exhaust Emission Guideline Development and Standard setting
- Air Pollution/Combustion Pollutants Modelling
REFERENCES


4. UNEP


POLLUTION FROM MOTOR VEHICLES IN GHANA
Kwaw Anaman
Mechanical Engineering Dept.
K.N.U.S.T.
Kumasi

INTRODUCTION
Dust, sulphur dioxide and other emissions from natural and anthropogenic sources are distributed by means of atmospheric transport phenomenon over wide distances. Once in the atmosphere, complex physical and chemical processes take place resulting in precipitations like acid rain or ozone formation.

Natural sources include vegetation, sea, volcanos, waste from biomass while anthropogenic sources - emissions caused by human beings - are associated with energy production, transportation, industry, domestic activities and agriculture. Emissions from vehicles, namely oxides of nitrogen, carbon monoxide, unburned hydrocarbons, particulates (ash and soot) come under anthropogenic sources.

In many parts of the world notably Los Angeles and Mexico City, emissions from vehicles have caused and continue to cause very serious problems. High emission concentration, high sunlight intensity and low levels of air movement have resulted in smog formation in these areas.

The increasing number of vehicles on our roads means increasing levels of noise — from engines and horns — traffic congestion and pollution of the atmosphere. Initially, in the 60’s and 70’s, the concern was mainly with smog resulting from the products of incomplete combustion of automobile fuels namely oxides of nitrogen and unburned hydrocarbon. In recent times, CO₂, a product of complete combustion has also become a subject of concern because of its contribution to the greenhouse effect.

In 1960, the State of California legislated against the motor vehicle and came out with testing procedures and levels of pollutants which will have to be met by vehicles in the State. The procedures covered the types of emissions to be controlled, (HC and CO), the sources of emission (exhaust, carburetor, crankcase and fuel tank), the test procedures, the instrumentation and test equipment to be used.

The background to this legislation was the smog which was experienced particularly around Los Angeles. Smog causes irritation to the eye and nasal passages, affects vegetation and has brought about economic losses in horticulture and agriculture. Smog is created by the action of sunlight on hydrocarbons in the atmosphere. The main source of hydrocarbons in the atmosphere is the exhaust gases of vehicles. Initially the aim was to reduce the total exhaust emissions to pre 1940 levels by 1980. The legislation was only against new vehicles as no requirement was made for existing vehicles to be modified.

At the time of the introduction of the legislation, it was believed that smog was caused by CO and unburned HC. Air-fuel mixture strengths were reduced to reduce the CO and HC output but the smog levels were unaffected. It was later discovered that the oxides of nitrogen (NOₓ) and unburned HC combined photochemically in strong sunlight to create smog. The US Federal Government followed with a legislation through the Environmental Protection Agency although
smog was not the primary concern in other parts of the US where the atmospheric conditions for its creation did not occur.

In the wake of the legislation introduced in the USA, the introduction of emission controls for motor vehicles has spread to other countries notably the developed countries. Africa and other developing regions are yet to introduce emission controls, apparently we have other problems which require immediate attention. The use of leaded fuels has been reduced significantly or stopped completely in Europe as a response to the demand to reduce the quantity of airborne lead particles in the atmosphere 90% of which are attributable to petrol consumption. In Japan and North America, lead has been removed from petrol because it poisoned the catalyst of chemical converters fitted to engines to reduce the exhaust emissions and not for environmental reasons related to lead itself.

In Ghana today, only leaded fuel is available on the market. What this basically means is that catalytic converters will be rendered useless in Ghana.

2.0 SOURCES OF POLLUTION

A vehicle contributes to pollution from several sources with unburned HC coming from the fuel tank vent and carburettor, from piston blow-by into the crankcase and leaks from fuel lines as well as the exhaust itself which put in addition CO, CO₂, NOₓ and particulates into the atmosphere. Crankcase emissions are dealt with by venting all crankcase fumes directly into the engine intake system to be burned in the engine cylinders. In Ghana, it is not uncommon to see vehicles which do not have any cover on their fuel tanks.

The major portion of the exhaust gas consists of nitrogen, carbon dioxide and water vapour. These are the products of complete combustion and are non-toxic. CO₂ emissions however contribute to the greenhouse effect and are therefore basically undesirable. Automobile exhaust gases also contain the following toxic components as a result of incomplete combustion.

**Carbon monoxide**: volumetric concentrations of 0.3% can result in death within 30 minutes.

**Oxides of nitrogen (NOₓ)**: The concentrations found in exhaust gases and in extremely polluted air can induce irritation in membranes.

**Unburned hydrocarbons (HC)**: when exposed to sunlight and nitrous oxides, they react to form oxidants which can be a source of irritation to mucous membranes.

**Particulates**: Fine solid matter e.g. soot.

The way an engine is used affects the completeness of the combustion process and therefore the exhaust gas emission. The drive cycle includes periods of acceleration, deceleration, steady state cruising and idling. Each of these periods have their own characteristic emissions. The diesel engine is low on HC and CO emissions but high on NOₓ and particulate emissions.

3.0 Emissions control

The major industrialised nations have been moving towards implementation of the stringent US exhaust emissions regulations. Compliance with this legislation is achieved by using emission control systems which incorporate close-loop-controlled catalytic converters. Some emission control methods such as increasing the air-fuel ratio and recirculating part of the exhaust through the cylinders reduces the CO and HC output, controls the NOx and does not
increase the fuel consumption. These methods are also inexpensive. Others which require catalytic converters to be added as additional units can involve large costs.

There are two basic methods used to alter the composition of the exhaust gases

- Engine design measures
- Exhaust gas treatment

3.1 Engine design measures.

Engine design measures include fuel metering – using the appropriate air-fuel ratio - and exhaust gas recirculation (EGR).

In the case of EGR, exhaust gas is led into the combustion chamber to reduce peak combustion temperatures. Higher combustion temperatures induce an overproportional increase in the formation of NOx.

Valve timing: Internal exhaust gas recirculation can be implemented using large valve overlaps, but at the cost of rough idling and increased hydrocarbon emissions.

Compression ratio: The higher the compression ratio, the better the efficiency but higher compression ratios also mean higher temperatures and therefore higher NOx emissions.

Combustion chamber design: Low HC emissions are achieved with a compact combustion chamber featuring a minimal area and recesses.

Ignition Systems: The design of the spark plug and its position within the combustion chamber, together with the spark energy, ignition timing, spark duration influence emission levels.

Crankcase ventilation:

The concentration of hydrocarbons in the crankcase can be many times that found in the engine’s exhaust gases. Control systems conduct these gases to a suitable point in the engine intake tract from where they are drawn into the combustion chamber for burning.

3.3. Exhaust Gas Treatment

Catalytic after burning

The catalytic converter is composed of a carrier substrate which serves as a base for catalytic material. The active catalytic layer consists of small quantities of noble metals (Pt, Rh, Pd) and is sensitive to lead. It is therefore essential that engines with catalytic converters are run on unleaded fuel exclusively. No meaningful treatment of pollutants takes place until the converter has reached an operating temperature of 250°C. Operating temperatures of approximately 400-800°C provide ideal conditions for maximum efficiency and extended service life.

4.0 Reducing vehicular emissions in Ghana

Basically, the reduction of CO2 and other pollutants in the transportation area can be achieved through the use of more fuel-efficient vehicles, less polluting fuels and through increased use of mass transit systems like tritos, buses and especially rail systems. The objective should be to reduce the amount of fossil fuels used per year and therefore the corresponding emissions.
Given the state of our economy and the prevailing income levels, only used vehicles from the developed world are affordable to the vast majority of Ghanaians. Most of these vehicles are 6 to 12 years old. These vehicles being old, are not of the latest technology (no catalytic converters) and their fuel consumption, oil consumption and emissions are relatively high.

In the foreseeable future, most Ghanaians will continue to depend on used vehicles and engines with their high fuel consumptions and emissions. In the light of this, the following options are relevant to reducing the amount of fuel consumed and therefore the amount of CO₂ and other emissions:

- encouraging the use of the more efficient and more durable diesel engine, especially for commercial vehicles like taxis and trotros, which consume the bulk of our petroleum products. Typically, the petrol vehicle consumes over 50% more fuel than an equivalent diesel vehicle especially in city riding. In terms of durability, the diesel engine lasts on the average twice as long between engine overhauls (in km terms).
- encouraging the increased use of mass transit systems like buses and rail systems, thereby reducing the amount of fuel/ person/unit distance from 50% to over 85%, depending on the system.
- promote the use of less polluting fuels like Liquefied Petroleum Gas (LPG) and investigate the use of alternative fuels like alcohol in taxis and trotros as well as private cars.

4.1 Fuel-efficient Vehicles

Diesel Engines

Under half-load operation (which corresponds to city driving conditions) the petrol engine uses about 50% more fuel than an equivalent diesel engine. The reasons are follows:

- Higher efficiency of the diesel engine at part load
- Absence of the throttle valve in the diesel engine. The throttle valve contributes significantly to the high part load fuel consumption of the petrol engine.

Generally, diesel engines are rated (power ratings) much lower than petrol engines. It is not uncommon to encounter a 2500cc diesel engine with the same power rating as a 1400cc petrol engine (e.g. 55kw) with the former being more fuel-efficient than the petrol engine. Currently, custom duties are based on the cubic capacity. No reference is made to power ratings and no differentiation is made between diesel and petrol engines in terms of durability and fuel consumption. Really, fuel consumption should be the yardstick for taxation and not the cubic capacity.

Since commuter buses and taxis form a large component of the vehicles on our roads and therefore use a major portion of the imported petroleum products, (they have high annual mileage), encouraging the use of diesel vehicles has the potential of cutting our fuel bills by 20% to 30%. In terms of greenhouse emissions, fossil CO₂ emissions could be cut by 20% to 30%. Other emissions would be cut down considerably. This could translate to between $60 million and $120 savings million in the national energy bill annually.

No taxi runs on petrol in Europe. It is simply not economical. Taxis run on diesel, a few run on LPG. The author is yet to see a diesel taxi in Ghana.
5.0 Service Life
Most of the used vehicles coming into the country are more than 5 years old and have covered over 100,000 km.

The average petrol engine can operate up to about 250,000 km whereas an equivalent diesel engine may be able to do up to 600,000 km without major overhaul. This is a direct result of significantly lower engine speeds and lower power capacity ratio which result in about half the thermal stresses and about a third of the dynamic loading in comparison to equivalent petrol engines.

The table below (Eastop and McConkey, 1993) shows that a 2.3 litres petrol engine uses over 50% more fuel in city driving than an equivalent diesel engine. A 1.6 litre petrol engine does 27.7 miles/gallon whereas the much bigger 2.3 litre diesel engine does 33.8 miles/gallon. This translates into 20% more mileage. The latter comparison is not even justified. The diesel/petrol price differential which has not been factored in the above considerations is an additional bonus to the diesel driver. In Ghana today, the more fuel-efficient and durable 2.3 litre diesel engine would be attracting more custom duties than the 1.6 litre petrol engine. Anyone who imports a fuel-efficient vehicle saves the country foreign exchange and should be rewarded and not punished. This anomaly needs immediate correcting.

<table>
<thead>
<tr>
<th>Engine Size (litres)</th>
<th>Power (Kw)</th>
<th>Power Capacity Ratio (Kw/litre)</th>
<th>Consumption in City driving (mpg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.30 (Petrol)</td>
<td>84 at 5300 rev/min</td>
<td>36.5</td>
<td>22.4</td>
</tr>
<tr>
<td>2.30 (Diesel)</td>
<td>49 at 4200 rev/min</td>
<td>21.2</td>
<td>33.8</td>
</tr>
<tr>
<td>1.60 (Petrol)</td>
<td>77 at 6000 rev/min</td>
<td>48.1</td>
<td>27.7</td>
</tr>
</tbody>
</table>

If we consider the diesel/petrol price differential in addition to the above factors, the petrol engine taxi driver will spend about 60% more than his diesel equivalent in fuel costs and emit 50% more CO$_2$ and other pollutants. His vehicle will attain less than half the service life of his diesel equivalent (in km terms). Since the diesels have significantly longer lives, the nation will have to contend with less material in our junkyards.

Given the superior fuel consumption and durability of the diesel engine, and also taking into account CO$_2$ and other emissions and the significant potential foreign exchange savings to the country as well as the big savings to operators, it is hereby recommended that

diesel cars and mini buses irrespective of the cubic capacities up to 10 years old should not attract any taxes whatsoever at the point of entry.

This measure, it is hoped, will encourage Ghanaians to import diesel vehicles in preference over petrol vehicles, thus saving Ghana substantial foreign exchange and reducing vehicular pollution.
6.0 Mass Transit Systems

One of the most effective ways of maximising the use of fuels and hence reducing fossil CO₂ and other emissions is through the use of mass transit systems such as commuters, buses and trains.

Apart from considerations of fossil CO₂ and other emissions, we need to develop our rail network in the country for the following reasons:

- Rail tracks have long service lives (over one hundred years) as opposed to roads which in Ghana do not last even 10 years.
- Efficient movement of goods (timber, cocoa, bauxite, petroleum products, food, mails, people etc.).
- Reduces the number of articulated and other vehicles on our roads leading to fewer accidents and longer lives of our roads.

Running rail transport has not been profitable anywhere in this world – except in recent experiments in the UK - but the industrialised world maintain very extensive railway networks because they are safe, fuel-efficient and therefore environmentally friendly and more importantly, rail networks make economies more efficient.

The government should therefore look at the question of modernising and expanding the rail system to cover at least the regional capitals of the nation. In particular, the development of an efficient railway system within Accra and between Accra and Tema will improve the traffic situation, reduce overall fuel consumption and pollution considerably.

7.0 Environmentally Friendly Fuels

7.1 Liquefied petroleum gas (LPG)

Liquefied petroleum gas is a mixture of propane and butane. The name is explained by the fact that the gas assumes a liquid state at pressures of 2 to 20 bar depending on the propane/butane ratio and the temperature.

Any vehicle equipped with an IC engine can be converted for operation on LPG. Generally emissions from an LPG engine, including CO₂ are substantially lower than those achieved with a gasoline engine, even one equipped with fuel injection and a close-loop-controlled catalytic converter. Liquefied petroleum gas contains no lead or sulphur compounds.

7.2 Alcohol as fuel (spark-ignition engines)

The finite availability of fossil fuels provides an impetus for devoting increased effort to development work on engines and injection systems capable of using alcohols, such as ethanol and methanol, as alternative fuels. Virtually the only place where ethanol is used as fuel is Brazil, a phenomenon explained by it being available locally. In the US especially in California, increasing attention is being focused on methanol, which also has benefits regarding exhaust emissions, namely reduced emissions of NOₓ and CO₂ along with lower levels of ozone and smog formation.
7.3 Hydrogen as fuel (spark-ignition-engines)

Pure hydrogen will oxidise into water. No CO\textsubscript{2} or other pollutants are produced in the process. In future when photovoltaic generators become affordable, solar (photovoltaic) electrolysis plants can be set up to produce fuel hydrogen from water.

Zero-emission vehicles (ZEV)

Zero-emission vehicles are battery-powered or solar-powered vehicles. The problem of pollution from vehicle exhaust in California is so severe that 2% of all vehicles to be sold in California starting 1998 should be ZEV. Gradually this figure should rise to 10% by 2003.

8.0 Standards and legislation on emissions.

Before we even think of standards and emission control, we should first start monitoring the air quality and traffic situation at critical points where the traffic congestion is high. This monitoring should take place over a minimum of ten years so that credible trends can be established. Also, the trend in the number of vehicles plying our roads and the total amount of fuel used for vehicular traffic should also be monitored. More importantly, the economic situation and the purchasing power of the average individual should be given due consideration. Before we start putting a ban on the importation of over-aged vehicles or used engines we have to be careful not to kill our economy. Used vehicles and engines have created a lot of jobs in this country at Kokompe, Magazine and elsewhere. I wonder how many of us here can afford new vehicles. Even new vehicles, unless they are fitted with close-loop-controlled catalytic converters, will not meet the US requirements. In Ghana’s case, simple measures such as diversion or rerouting of traffic can do the trick.

Emission control and standards should depend on the particular environment under consideration. In other words, we cannot import the Californian standards or the Japanese requirements wholesale into this country. Our standards should take into consideration the road network, number and average age of vehicles and especially the total amount of fuel consumed per year for vehicular traffic. By comparison, the number of vehicles in Berlin—which is a little bigger than Accra—is about five times that of the whole of Ghana. Really we should be comparing the amount of fuel used and the average age of the vehicles and not the number of vehicles.

In industrialised countries, visible smoke is a traffic offence. Road users will normally inform the police of any vehicles emitting visible smoke. Particulates from vehicles in certain concentrations can cause tumours in the lungs. Exhaust emissions can have effect on plants, humans and buildings depending on the concentrations and duration of action.

We need to begin modestly and tread cautiously but progressively. Nowhere in this world have emission standards been static. For example, a modest start can be made by legislating against visible smoke and unnecessary blowing of horns.
9.6 Conclusion and recommendations

As the economy improves and more vehicles are imported into the country, vehicular emissions and their effects on humans are going to assume important dimensions. In the foreseeable future, we will have to concentrate on limiting the increase rather than reducing vehicular pollution in seriously affected areas.

Before setting standards or legislating on emissions, it is essential that the air quality at most affected areas are monitored, trends established and the potential health implications assessed. The quality of the fuel from our refineries should be monitored on a continuous basis and corrective measures taken where necessary. In some cases, simple traffic diversion, or restriction in vehicular movement will improve air quality considerably.

The use of catalytic converters requires unleaded petrol. The refineries will have to start producing regular petrol in the very near future otherwise Ghana will not be able to benefit from the catalyst technology.

Encouraging the increased use of the diesel engine through custom duties waivers especially for taxis and mini buses as well as improving and expanding the rail network will reduce the amount of fuel consumed and therefore conserve foreign exchange, reduce emissions, increase the lives of our roads and reduce accidents.

LPG and other less polluting fuels also offer a chance at reducing vehicular emissions.

Legislation on exhaust emissions require progressive reductions to be made in HC, CO and NOx content of exhaust gas from vehicles. A modest start at setting standards is to legislate against visible emissions (smoke).
REFERENCES


APPENDICE
ICS-UNIDO WORKSHOP
EVALUATION QUESTIONNAIRE

TITLE: COMBUSTION DIAGNOSTICS AND OPTICAL TECHNIQUES

A. ORGANISATION

Participants were highly impressed about the publicity, announcement and pre-workshop information process. They found the scientific programme, practicals and the lectures very useful and well presented by the lecturers. The case studies provided by the Oil Refinery, the mining industries and the Environmental Protection Agency in Ghana about the combustion processes and monitoring technique were very informative. The questions and answer (discussion) sessions were very lively. The participants also found the visit to some industries (Tema Oil Refinery and the Valco Aluminium Smelting Plant) very useful.

However the participants were of the view that a much smaller working group than was used, would have made the laboratory (practical) sections more interesting and beneficial.

B. DURATION OF PROGRAMME

Most participants thought the number of days used for the workshop was right. However a good number of them were of the view that the programme of activities for the days were too loaded. This did not offer them enough time to interact with the lecturer and other participants from different countries.

C. TRAINING FACILITIES AND HOTEL

The general consensus was that the hotel accommodation, meals, refreshments and lecture/training rooms were excellent.

D. ORGANISER'S RESPONSE TO PARTICIPANTS NEEDS

The participants gave the organisers high marks and commended them for the efficient and able manner they addressed their needs and problems any time such problems did arise.

E. OVERALL PROGRAMME ORGANISATION

The overall impression was that the workshop was excellently organised. The participants were satisfied with almost everything that went on at the workshop.

F. Most participants said they were ready to recommend to other scientists from their country and institution to attend similar activity in the future.
While most of the participants said they found almost all the activities useful, about 80% said they found the practical sessions and the case study provided by the local industries in Ghana most useful.

Most participants said they gained a lot from the practical sessions. However some thought a smaller working groups for the practical sessions would have been preferred.

The visit to some industries in Ghana was most appreciated by the participants.

Participants generally agreed that the workshop was very beneficial. They said the workshop offered them the opportunity to acquire more than basic knowledge in Laser Technique and its application. It also helped enlightened them on combustion processes and hazards and how to detect and minimize the effects of these pollutants.

A better understanding of combustion systems and laser and optical diagnostics technique were gained.

They expressed the desire to disseminate the information and knowledge acquired during the workshop to their colleagues, students and government officials through seminars and lectures. Some were so motivated that they said they were going to prepare a Comprehensive Report about the worship to their Government so as to help them research into some of the combustion problems in their countries. Other also expressed the hope to build basic optical monitors for monitoring certain emissions in their country.

The participants also suggested a number of programmes and future activities ICS could pursue to help with the technological and scientific advancement in some of their countries. Among these were workshop on

- Fibre Optics and Communication
- Meteorology and climate change
- Electronics and Data Processing

G. EVALUATION OF LECTURERS AND SPEAKERS

According to the participants the lecturers and speakers, both resident (local) and international, were excellent. The presentations were well delivered. Course materials were also excellent. Questions were well handled by the lecturers. The questions and answers (discussion) sessions were very lively.

COMMENTS

The workshop was very useful, for, it did open the way for more interactions between research institutions and the industries.
RESOLUTIONS ADOPTED BY THE PARTICIPANTS AT THE INTERNATIONAL WORKSHOP ON COMBUSTION DIAGNOSTICS AND OPTICAL TECHNIQUES

INTRODUCTION

We the participants of the above workshop having deliberated (through lectures, laboratory sessions, and industrial visits) on various topics such as Combustion Diagnostics, Optical Measurement Methods, Absorption and Emission Spectrometry, Laser Probing of Combustion, and Air Pollution due to Combustion, have realised the tremendous potential Laser and Optical Techniques (LOT) offer in industrial applications for combustion - and environment-related issues.

We also appreciate the support of the International Centre for Science and High Technology (ICCS - Italy), UNIDO (Ghana), Tema Oil Refinery (TOR) and other companies in the petroleum-related sector (Ghana).

ISSUES IDENTIFIED
We have noted with serious concern that:

1. Research and Development in combustion systems, locally and within the African Region, is scanty and uncoordinated

2. Combustion processes, both industrial and domestic, lead to the emission of pollutants into the atmosphere

3. The advantages that laser and optical techniques offer as a tool in combustion and environmental diagnosis is woefully underutilised by our industries

4. There exists a lack of adequately trained manpower, and insufficient facilities within the public and private sector for atmospheric pollution studies.

RESOLUTION

Taking cognisance of the above-mentioned concerns, and bearing in mind our objective to forge and sustain linkages between Universities, Research Institutions and Industry for Laser and Optical applications in combustion - and environment related issues, we the participants at this workshop hereby resolve as follows:

1. Applied research projects should be developed based on need-driven projects identified, designed, planned, and implemented jointly with industry and relevant sector ministries

2. Projects must focus on enhancing understanding of combustion processes and atmospheric pollutant dispersal through experiments, simulation and modeling.
3. Thematic plans to be developed should include the following key issue areas: Burner Design, Performance, Evaluation and Improvement of Combustion Process, Atmospheric Emissions and Measurement of Greenhouse Gases.

4. Scientists, Engineers, Technicians and Students should be trained and developed for the establishment of local expertise in combustion, emission control and laser and optical techniques.

5. Supplementary equipment and facilities should be provided to the Laser and Fibre Optics Centre (LAFOC) to facilitate the implementation of identified joint projects.

6. An Oversight Committee should be set up to serve as co-ordinating body for national and international stockholder institutions, to plan follow-up activities and to source funding for projects and programmes, and explore opportunities for regional cooperation.

7. Analysis and Evaluation of alternative transportation methods to reduce air quality emission should be undertaken.
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