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The Institute of Physics

COMBUSTION PHYSICS GROUP NEWSLETTER

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1 COMBUSTION PHYSICS GROUP COMMITTEE 2000/2001

1.

Chairman:	Dr M Fairweather	University of Leeds
Vice-chairman:	Dr Alex Taylor	Imperial College
Secretary:	Dr G. Hargrave	University of Loughborough

Ordinary Members:

Mr J. Allen	Scion-Sprays Ltd
Dr P.J. Bowen	Cardiff University
Dr R. Boyce	Rolls Royce
Dr P Cadman	University of Wales, Aberystwyth
Mrs Catherine Goy	PowerGen plc
Dr C. Lea	HSL
Dr Mike Ross	Alstrom
Dr P. Rubini	Cranfield University

Co-opted Members:

Dr A. Jones	Imperial College
Dr D Towers	Heriot Watt University
Dr P. Stephenson	Innogy

2. EDITOR'S CORNER

The IOP have started issuing regular policy updates from Headquarters. I hope to extract some regular News items from them for this Newsletter. There are shown below under 'News' It is 2003 when this Newsletter now appears. It was hoped that this letter would have appeared in Autumn 2002 but a number of difficulties prevented this. Anyway I hope it was worth the wait!

Once again I am making a plea for articles, conference reviews etc for this Newsletter. A sum of £50 is available for articles by bonafide research students on topics connected with combustion. I am prepared to be flexible on the type and length of such articles so supervisors please encourage your students to write one! In addition it would be nice to have articles by retired members on their thoughts reminiscences of working in combustion in the past – difficulties encountered, meeting scientists, historical perspectives on research laboratories- the list is almost endless. If anyone has any ideas for articles I would be pleased to hear from them. ---Phil Cadman

3. NEWS AND ARTICLES INVOLVING COMBUSTION

The IOP Combustion Committee intends to introduce in 2003 a prize of £500 for the best PhD thesis in combustion. Applicants should send in the first instance, an extended abstract (~1000 words), together with a supporting letters from their supervisor and external examiner to the Editor of this Newsletter (address at the end) before June 30th 2003. PhD theses from 2003, 2002 and 2001 can be considered for this prize.

IOP's Career Break Support

- The Institute's Career Break Grants help members to stay in touch with the wider physics community.
- Contributions towards attendance and associated costs are available.
- Members can apply by going to

<http://careers.iop.org/resources> Or by emailing cbg@iop.org

Career Break Rates for Conferences

- Members can attend all Institute of Physics conferences at a reduced rate.

Reduced Membership Subscription Rates

- Members on a career break are entitled to a reduced membership subscription rate, which is currently just £10.
- Email membership.iop.org, including your membership ID number in the text, to qualify for this rate.

Developing countries to gain from carbon trading fund

Rural communities in the worlds poorest nations will be able to earn income by using their forests and agricultural land to sequester CO₂ , under a plan announced by the World Bank- (Nature **470** 4 ,7th November 2002)

Burning Peat sparks global warming fears

Burning peat bogs in Indonesia are releasing massive amounts of CO₂ into the atmosphere, in a repeat of the environmental devastation that made headlines around 5 years ago. (New Scientist 11, 9th November 2002)

US goes underground in scheme to bury greenhouse gas (Nature **420** 353, 28th November 2002)

Industry views on future energy policy published (DTI press release 27th November 2002)

Filters for Diesel Engines (Environment Business Magazine November, 14, 2002)

Particulate control for Power Stations (Environment Business Magazine, 14 November 2002)

Ireland advised to centralise energy strategy A major new document on research strategy in Ireland urges the creation of an oversight body for research based at the centre of government. Recommendation comes from Higher Education Authority.

Energy Supply: How secure are we? (House of Lords Select Committee Session 14th report – TSOL, 2001-2)

Ratifying Kyoto Postnote No 176 (Parliamentary Office of Science and Technology, April 2002)

The Energy Review – A performance and innovation unit Report, Cabinet Office, 14th February 2002)

Energy –Its impact on the Environment and Society (DTI, 25th July 2002)

Carbon Sunk Since 1996 over 5M tonnes of CO₂ have been stashed below Sleiper Field in the North Sea. (New Scientist, 21th September 2002)

EC concludes debate on the security of energy supply (Nuclear Engineering International, 5 August 2002)

Government urged to help British Energy Professor David King urged Ministers to help troubled nuclear power company by exempting it from climate change levy (Financial Times, 2, 16th September 2002)

2002 Digest of UK energy statistics and energy consumption (DTI, 25th July 2002)

Ofgem recommends climate change policy shake-up for UK to meet greenhouse gas emission targets, including compulsory emission trading and imposition of carbon tax. (Financial Times, 4, 8th August 2002)

Power without Pollution: an R & D strategy for electricity generation with near to zero emissions (Foresight Energy and Environment report DTI, 27th March 2002)

EU emissions stabilise . CO₂ emissions have levelled out between 1999 and 2000 (Environment Business Magazine, 8, June 2002)

Report claims Kyoto will stifle economy (Environment Business Magazine 7, June 2002)

Under ground gas storage could be key to meeting Kyoto targets (Cordis, Issue **196** 10, 6th May 2002)

Canada pushes for Kyoto Concessions (Cordis, issue **197** 21, 20th May 2002)

Japan signs up for Kyoto (Nature **417** 478, 30th May 2002)

4. REPORTS ON MEETINGS

4.1 Minutes of the Annual General Meeting of the Combustion Physics Group of the Institute of Physics

This was held at The Institute of Physics, Portland Place, London, on the 9th October 2002 and consisted of:-

(i) Minutes of the Last AGM

The minutes of the last AGM, held at Advantica Technologies Ltd. on 20th September 2002, were read and approved.

(ii) Matters Arising

David Towers had requested assistance from the Combustion Physics Group (CPG) Committee in organising the Photon02 Meeting held in September of this year, and such assistance had been provided.

(iii) Chairman's Report

The Chairman, Dr. Fairweather, reported that the last year had again been very active for the Group. The CPG had held three meetings in the last 12 months, and two well-attended conferences had been organised. A joint "Work-in-Progress Poster Meeting", in collaboration with the Combustion Institute (British Section) and the British Flame Research Committee, had been held at Queen Mary, London on 17th April 2002. This meeting focussed on non-laser diagnostics, two-phase reacting flows, and the combustion of syngas and biomass fuels. A complementary meeting on "Optical Techniques for Combustion" was held at the Photon02 Meeting in Cardiff between 2nd-5th September 2002.

A number of other meetings had been co-sponsored by the Group, benefiting CPG members through reduced admission rates. These included the Combustion Institute (British Section) "Autumn Research Meeting" held at Cranfield University on 16th-17th September 2002, and the "Advanced Sensors and Instrumentation Systems for Combustion Processes" meeting which was held at the IOP on 9th October.

Dr. Cadman had produced a full Newsletter for Group members in February of this year, with a further Newsletter due shortly.

The Committee had contributed to a number of IOP- and EPSRC-led consultations and briefing documents on sustainable energy supply. Further to discussions with the EPSRC, reported in last year's Minutes, a list of possible referees for combustion research proposals had been compiled and submitted to the EPSRC in November 2001 by the IOP CPG together with the Combustion Institute (British Section) and the Coal Research Forum.

A £500 travel grant had been awarded to assist a student working for a member of the Group in travelling to the 29th International Symposium on Combustion held in Sapporo, Japan between 21st-26th July 2002. A similar travel grant was also awarded to a group member, and it is anticipated that this will be paid in due course.

Highlights for the coming year include a spring 2003 meeting on "Ongoing Requirements for Combustion Research: A UK Perspective", and a meeting on "Waste Disposal" being organised jointly by the IOP Environmental Physics Group and the CPG to be held at the IOP 2003 Congress that is taking place at Heriot-Watt University, Edinburgh between 23rd-26th March 2003. The CPG is also co-sponsoring the "4th International Seminar on Fire and Explosion Hazards" to be held in Londonderry between 8th-12th September 2003.

A sub-committee of the CPG had also been formed to look into the award of prizes by the Group, and this will hopefully lead to the first awards being made in the coming year.

(iv) Secretary's Report

The Group Secretary, Dr. Hargrave, could not be present at the AGM, although the main items of his report were read out by the Chairman and are covered in Section 3 above. Membership figures for the

last year show that the Group had 174 members. The Group's finances are also in a healthy state, with the current account showing a balance of £8166.

(v) Election of Officers and Ordinary Members of the Committee

No Officers of the CPG were up for election this year, with all eight of the Ordinary Members of the committee also still being within their 4 year terms.

Subject to joining the IOP, Peter Stephenson (Innogy) was elected as an Ordinary Member following his year as a Casual Member of the Committee.

The co-option of Alan Jones (Imperial College) was extended to allow him to fulfil his previously identified role. The co-option of David Towers (Heriot-Watt University) was also extended to allow him to provide valuable links with the IOP Optical Group and the Applied Optics Division as a whole.

(vi) Any Other Business

Prof. Weinberg raised the issue of recruitment of IOP members to the CPG and, in particular, targeting attendees at meetings such as that being held at the time of the AGM (Advanced Sensors and Instrumentation Systems for Combustion Processes). Dr. Fairweather responded that such initiatives were being explored by the Committee, but would raise this issue at the next Committee meeting.

4.2 Optical Techniques in Combustion – A 1-day Conference at Photon02.

- Dr D Towers, Department of Mechanical and Chemical Engineering, Heriot-Watt University, Riccarton, Edinburgh EH14 4AS

A full day of the Photon02 conference was devoted to optical techniques in combustion. The programme consisted mainly of academic papers with one session of contributions from commercial developers of optical instrumentation. Heiner Voges of La Vision provided an excellent overview of both particle based and spectroscopic based diagnostics. The talk was exemplified by many examples from their own instruments. The academic papers were mainly devoted to spectroscopic based combustion sensors. This was a marked difference compared to similar conferences held in the late '90s where an approximately equal division of particle and spectroscopy based work was being reported. The other commercial instrumentation developers, in contrast, concentrated on particle-based diagnostics. Perhaps this trend is indicative of the difficulty in commercialising spectroscopic based combustion diagnostics, either because of the technical difficulties in quantifying measurements from hostile environments or because suitably qualified staff are not available in the companies who wish to be end-users. The meeting was attended by 25-30 people with many high profile names from the UK research base. The quality of papers and verbal presentations were good and generated interesting and lively exchanges.

The academic papers spanned all aspects of optical combustion sensing: sources, detection schemes, data reconstruction and processing. Three papers were presented from Cranfield University covering the area of spray diagnostics, including laser sheet drop sizing. Applications of these methods to both automotive and gas turbine sprays were presented including a discussion of how the data may be used to understand the important mechanisms responsible for gas turbine instability. Oxford University presented two papers regarding non-linear optical techniques. Firstly, laser induced thermal grating spectroscopy was demonstrated for temperature and pressure measurement in a methane/air flame. Secondly, a new widely tuneable, single longitudinal mode laser was described and performance advantages demonstrated in four wave mixing experiments. UMIST presented two papers where laser diodes were employed for illumination in absorption and fluorescence modes. Diodes at 1700nm are coincident with a weak gasoline absorption band for vapour phase tomographic imaging, whilst at 404nm fluorescence is observable from liquid gasoline. The semiconductor laser theme was extended in work at Huddersfield University where near infra-red lasers were described for detecting (by absorption) the concentration and temperature of a wide range of combustion products and intermediaries. Naturally occurring chemiluminescence was employed by workers at Imperial College where simultaneous detection of multiple radicals (spectrally discriminated) provides quantitative measurements of heat release and equivalence ratio in reacting flames. Finally, high speed scanned

imaging of burnt / unburnt gas components allowed Leeds University to reconstruct the full three-dimensional shape of the reaction front in a turbulent combustion event in order to understand fundamental issues of flame front wrinkling and the relationship with burn rate.

A book of extended abstracts from the entire Photon02 conference has been produced under ISBN 0-7503-0916-4 for the interested reader. The organisers wish to thank the session chairs, contributing authors and the attendees for making the conference an enjoyable and topical day.

4.3 Combustion Symposium Summary ‘A Diary from the Rising Sun’

- Phil Bowen, Cardiff School of Engineering, Division of Mechanical Engineering, Cardiff University, Queen’s Buildings, The Parade, PO Box 925, Cardiff CF24 0YF

Though a committed traveller, had strange feeling about this conference trip – Japan has never featured highly on my prioritisation list, but had this feeling that I was going to be pleasantly surprised when I got there. This in fact turned out to be the case, having spent a very pleasant day wandering around the sights in Tokyo whilst in transit on day 1 – Rinzi neon lights, etc. - awaiting my connecting flight to Sapporo. Rather expensive, though not significantly more so than the UK I guess. First impressions were very positive.

The first familiar face I bumped into amongst a sea of oriental faces in the departures lounge at Narita was another Welshman (not sure what you consider yourself Alan, but few years spent in Merthyr in your youth would be sufficient to be considered by Mark Hughes I’m sure, so we’ll lay claim) Alan Williams. Everyone bit edgy as flight delayed and nobody sure who’s waiting for which flight in the throng of people at Gate 36/37. Anyhow, all works itself out in the end, and we all arrive in Sapporo just in time for all the eating places to shut ! Get few sandwiches from equivalent of local SPAR – appear to open later than 10pm here - and off to sleep off my jet-lag.

Notwithstanding the generous IOP contribution to my costs, overall trip still a bit expensive, so booked into cheapest hotel on recommended list. Still £50-ish per night though. However, online Internet in coffee area, so not as bad as anticipated, though toilet door in my room has to open outwards to save space. It’ll do as home for the next week!

First day rather adventurous, and find out a bit more than I would have liked about Japanese culture. Manage to walk my way through the 8ft x 4ft plate glass hotel door lunchtime, getting showered in glass in the process. Attendee from Sydney University observes this from reception, and comes over to see if I’m OK. After seeing that not much (personal) damage incurred, we start chatting about combustion, whilst receptionists pick glass splinters out of my arms, and he asks in due course what my presentation is about : - ‘Hazards’ I reply without thinking, much to his amusement ! Managed to negotiate my way out of paying for it – which would have consumed the grant – after some considerable debate with hotel staff, and as a last resort the mention of doctors, headaches and compensation!

Other interesting observations from day one are Japanese heated toilet seats, ultra-efficient hand-driers, the unacceptability of jay-walking, and the general pleasant and hospitable nature of the Japanese people. All augurs well – I like this place!

So much for the cultural experience – guess that’s not quite why the grant was awarded ! - onto the academic aspects. Despite the late arrival, manage to get breakfast in and make the 8.30 plenary given by Sebastien Candel. Very good summary of current issues concerning combustion instability and control - obvious emphasis on gas turbines - enlightened by some very impressive graphics including pressure-induced ‘Pagoda’ flames aptly renamed ‘Japanese Temple’ flames for the purpose of the presentation. As Chair (think its Forman Williams, but can’t be sure from the back of an enormous lecture room) points out, a typically French artistic flavour!

For the first time at a conference (it’s the guilt factor of the IOP award), I actually attend a talk at every session – 12 in all - which involves short walk between 2 hotels – not much inconvenience, and conference is up and running smoothly. Bump into some familiar faces and catch up with people

during breaks. On first day lectures, my selection obviously governed by my research interests, but overall feeling of starting to relax after the rigours of 'end of semester' back home ('wish I'd given that referral exam paper a final check before leaving though!'). Good conferences always recharge my research batteries after the rigours of the academic year, but the Symposium I find particularly inspiring, offering such a diverse range of subject areas, as well as personalities of course.

My oral presentation is not until Friday, with Cardiff WIP posters I'm attending displayed on Thursday and Friday – hence, my duties are rather 'back-ended'. Prioritise presentations I want to attend, with Tuesday sessions broadly taking me back and forth between engine research (diagnostics, modelling, pollutants), laminar/turbulent flames, two-phase/spray contributions, hazards and combustion instability sessions. Use my usual prioritisation methodology, with single asterisk for students back home to chase up when I return - system serves me well yet again.

Spend the next few days in similar vein, trying monitor research progress in areas relating to ongoing research projects back home, whilst trying to fit in others not usually in my mainstream, which for one reason or another catch my eye in the abstracts list.

Wednesday was an interesting day for those with interests in combustion hazard work. Toshisuke Hirani started the day with a plenary session on Combustion Science for Safety. Technically, a rather elementary talk, basically an overview of how combustion safety science has evolved in Japan through the National Research Institute for Fire/Explosion Disaster (NRIFD). Interesting for national, organisational and cultural comparisons though.

Continuing the hazard theme through Wednesday was the Special Session on Sept. 11th. Prof. Quintiere, gave an invited paper concerning the fire aspects of the disaster, with Prof. Georgy Makvhiladze providing the second invited paper concerning analysis of the fireball component of combustion. This was followed by a discussion session, with about half a dozen groups adding more specific points emanating from related research programmes, including NIST (US National Institute of Science and Technology) who were leading the US government technical enquiry from I could gather, and who had received the odd hint of criticism from previous speakers. Couple of points I found of interest were the dominance of the office/building materials in the fire event compared with the aviation fuel, and that a simple phenomenological model had allowed Prof. Quintiere to predict the time-to-collapse of each building reasonably accurately (published in Journal of Fire Science apparently). I had submitted a brief contribution for the discussion session, commenting on the necessity to predict the initial source term of the fuel:air cloud and the subsequent combustion rate through it, a point consolidated by Prof. Dryer. I came away with the impression that UK Ltd. was very well placed in terms of expertise and knowledge-base concerning such large-scale hazard quantification.

Attended the conference banquet on the Thursday evening. Always caught in two minds as to whether to pay out to attend these, but on this occasion, was glad I did. Arbitrarily chose my seat, and ended up sat on table with a mix of Americans from NASA, NIST and some of Forman Williams' research students. Had been interested in Greg Lineris' talk on chemical suppression that afternoon and wanted to quiz him further, so it was welcome surprise to find myself sitting next to him and his wife (who believe it or not, was actually familiar with Wales, having visited Cardiff as a student). No, didn't bother Greg with work talk at the dinner, but made the contact which I guess is part of the *raison d'être* of these conferences. Interesting musical entertainment between courses, with 3-stringed Japanese guitars attempting renditions of Western popular music, with table entertainment of 'first to name that tune !'. Some were rather well disguised, it has to be said.

The concept of 'Pulse Detonations' grabs my attention in one of the sessions later in the week – seems to be rather a theme at this Symposium. Done a bit of work on Pulse Combustors over past few years, but not sure on this variation (apart from obvious). Brief chat with Geraint Thomas over few beers at the Farewell Reception gives a bit more insight, but one I'll have to read up on back home.

Friday morning plenary lecture probably one of the more candid I've heard for some time, yet I guess I should have expected nothing less from a familiar face - our EU assessor at Cardiff - Klaus Hein.

Though bit of a debate in coffee session following regarding the applicability of such 'politically-oriented' talks to a mainly technical audience, personally think it does no harm to move into reflective

mode, and consider the implications and reasons behind our research and the political impact now and again. Talk took us through the future world energy requirements in relation to current and future demand, and Klaus pulled no punches in clearly identifying the American role in these challenges (prompting a post-presentation comment from Prof. Fred Dryer 'Yes, America does have a policy on the environment, and has done for the last 20 years !).

The other interesting reflection was on how sessions at the Symposium have changed broadly in sync. with societal/political developments since the inception in 1928, for example pollution only really being introduced in the late-sixties/early-seventies, and microgravity combustion around same time. The special session on Sept.11th may be referred to in similar reflective talks at future symposia I guess?

Couldn't have timed the finish of the Symposium better, it coinciding with a traditional Japanese firework evening – I'm sure there's a cultural reason for the celebrations, but haven't read up in my introductory notes. Was very impressed with Friday night out in Sapporo, with all ladies dressed up in traditional Japanese costumes (the Cardiff ladies from Splott dressing up in traditional Welsh costume somehow wouldn't have quite the same appeal !).

One thing to say regarding future IOP grants, as decided at last committee meeting before I left, don't sign the cheque until the summary has been submitted. Realise now writing this on my laptop on the flight back home, wouldn't be doing this without the financial incentive, and its far easier to write while fresh in the memory, rather than trying to understand scribbled notes in a month or so time. ****

Stay at airport hotel on final evening with connecting flight out to Osaka early Sunday morning. Whilst waiting in the 'Check-In' queue, bleary eyed at 6.45am, a familiar voice from behind me asks 'is this the right queue for Narita flight'. Turning around I find Alan Williams again, first familiar face I see on outward journey, and last 'Combustion' face I see on way back. Sort of ties up my diary rather neatly. Hope the G&T settled the nerves for the flight, Alan.

So here I am a few months later, still not having sent off this summary, and Phil (Cadman) and our financial division at Cardiff chasing me hard for a IOP Combustion Group Newsletter contribution, and repayment of my financial advance for Sapporo respectively. My time's up! Given myself half hour on train up to visit industrial placement student at Nissan (Sunderland) to now try to remember my scribbled notes from the summer – I now appreciate why my students complain at my review notes on theses and projects !

4.4 **29th International Symposium on Combustion, 21-26 July 2002, Sapporo, Japan.**

Conference Review—Catherine Gardner, Research Student, Department of Physics, University of Wales, Aberystwyth

As a conference novice I was very excited to learn that I was going to Japan to present a poster at the 29th International Symposium on Combustion and although the journey from Aberystwyth was long my supervisor and I arrived in Sapporo in good spirits, looking forward to the week's events.

On Sunday I had the opportunity to have a good look around the city and really get my bearings!

Sapporo is large compared to the small town of Aberystwyth, but unlike some big cities it did not have that threatening aura, maybe it was the way they played bird song out of speakers on the street! I also found it to be exceptionally clean and tidy compared to a lot of British cities. In the afternoon we registered, which was quite painless, and had a good read through the abstracts for the talks and poster sessions. We then made our way to the welcome reception, where I organised how large the conference actually was. In total there were more than 850 delegates from around the world and over 35 representatives from the UK. With more than 20 accepted papers and a host of poster presentations between them, the British combustion community had impressive representation. I seemed to make friends almost immediately with several people and saw many people meeting up with others they hadn't seen for a while. The food had a really good mix of traditional Japanese and slightly more western styles so everyone could refuel.

Monday saw the sessions begin and myself run around from talk to talk! There was a broad range of topics on offer, which provided a newbie like me, the perfect opportunity to learn about subjects that I

had, up until then, yet to encounter. I particularly enjoyed many of the talks in the turbulent combustion session and found the techniques raised in the reaction kinetics presentations worth further consideration. I found that the sessions gave me the incentive to investigate many new topics further.

One paper that I found particularly interesting was presented at the internal combustion engine session by M.S. Wooldridge and concentrated on the modeling of two different effects – chemical and mixing effects on auto-ignition a subject that I am particularly fond of. The idea that two codes could be interchanged according to the conditions to provide a more realistic simulation appealed to me, partly because some of my own work concentrated on adding a physical parameter to a one dimensional kinetics scheme.

Other papers that captured my attention were two by Tim Lieuwen who had an interesting approach to investigating turbulent pre-mixed flames through the interactions of acoustic waves with the flame by measuring and organized the scattered waves from a turbulent flame bombarded by a coherent wave form. This technique gave information about the surface of the evolving flame front and the effects of small scale perturbations on the mass burning rate and temperature gradient across the flame.

Throughout the week I also had the chance to take a look at the poster sessions and was impressed by the overall standard of the work on offer and how it had been presented too, as a presenter I was very pleased to see how relaxed the atmosphere was to allow discussion in a non-threatening environment and I had a very nice chat with a guy, who's name escapes me, about vortex production.

Monday also saw the start of the beer festival! So my supervisor and I headed to the town park for a quiet drink after a hard day's work. We soon made friends with some of the local medical students who, like the people on the table next to us, were eager to practice their English. The tent was run by the Kirin beer company and to our surprise the medical students left and donated what appeared to be a 4ft Perspex vertical shock tube of beer – waste not want not!

On Wednesday we had a half day tour to get out of the city to North Horse Park, which, as the name suggests had a distinctly horsy theme! And even though the weather had taken a turn for the worst the whole afternoon was a great success, for me this was mainly due to the life-size 'ride-able' mechanical horse.

Included in the excursion were a range of activities and a do-it-yourself barbeque lunch, which was great because you could eat as much or as little as you pleased and, needless to say, cooking using chopsticks was quite an interesting exercise especially with beer involved – a bad combination! The entertainment was available after lunch as well, so with plenty of beer inside for Dutch courage the balloon archery and laser shooting were given a go. However, the most joy was obtained from the golf carts that you were allowed to take out even after consuming what could only be described as a 'skin full'. Racing and bumper cars seemed to be the order of the day, although for a more sedate evening you could sit and enjoy some classical music and opera performed live.

Thursday arrived much quicker than I'd imagined and it was time to present my poster to the masses! After a few minutes of panic I settled down and was very pleased when people started to take an interest in my work and enjoyed the opportunity to meet more of the delegates – on the whole it was a very satisfying day and challenging day.

The evening event was a traditional Japanese banquet and although I did not go myself – the call of Karaoke was too great – I heard some good reports about the food and the company. On the whole the conference was very well organized, and a good time (both scientifically and socially) was had by all that I met. I will certainly be booking my ticket for Chicago in two years time!

5. FORTHCOMING MEETINGS - IOP SPONSORED MEETINGS 2003

A one day meeting entitled ‘**Ongoing Requirements for Combustion Research a UK Perspective**’ will be held at the **IOP (Portland Place London)** on Thursday April 24th 2003 starting at 10-30AM. A number of experts will outline their perspectives on this topic.

Fees Members £25, non members £48, students £15 to include lunch. More details and application forms can be obtained from Dr G Hargraves, Secretary IOP combustion Committee –address at end of this Newsletter)

IOP Congress Heriot Watt University Tuesday 25th March 2003 A Symposium on ‘Waste Management ‘ details see Website congress.iop.org, or email to congress@iop.org
Young Researchers Forum September 2003 more details from either Dr R Boyce or J. Allen, Addresses at end of this Newsletter.

6 AN OVERVIEW OF THE STATE OF THE ART IN GAS EXPLOSION MODELLING

-Dr H S Ledin, Health & Safety Laboratory, Harpur Hill, Buxton, Derbyshire, SK17 9JN

Introduction

HSL have recently undertaken a wide-ranging review of the state of the art in the modelling of gas explosions, on behalf of the UK Health & Safety Executive (Ledin, 2002). The aim of this review was to inform the Hazardous Installations Directorate about the current status and future direction of gas explosion numerical models presently in use. Gas explosions are of course a major hazard in both the on-shore and offshore environments.

The 1974 explosion at the Nypro plant at Flixborough is one of the most serious accidents to afflict the chemical processing industry. The explosion at Flixborough was caused by the ignition of a flammable cloud containing about 50 tons of cyclohexane, the cyclohexane release was probably due to the failure of a temporary pipe. The blast has been estimated to be equivalent to about 16 tons of TNT, with the result that 28 people were killed, 89 injured, the plant was totally destroyed, and damage was caused to nearly 2000 properties external to the site.

In 1988 on the offshore platform Piper Alpha a small explosion in a compressor module caused fires, which resulted in the rupture of a riser. Most of the platform was subsequently destroyed by fire, causing the death of 167 people. The over-pressure generated by the initial explosion has been estimated to be only 0.3 bar.

HSL’s review describes empirical models, phenomenological models and Computational Fluid Dynamics (CFD) based models. Empirical models are the simplest way of estimating deflagration over-pressures. These models contain correlations and contain little or no physics. Phenomenological models are simplified models, which represent the major physical processes in the explosion. CFD models involve numerical evaluation of the partial differential equations governing the explosion process and yield a great deal of information about the flow field.

It should be noted that the work is restricted to numerical models of deflagrations, rather than detonations.

The complete report, which stretches to over 90 pages and contains more than 80 references, can be accessed from HSE’s web-site. A brief overview of the content, and in particular the main conclusions, are given overleaf.

Objectives

1. To identify organisations involved in gas explosion research in the U.K. and Europe.
2. To survey these organisations, to determine their areas of current and proposed work.

3. To collate their responses in a report, which also provides an up to date literature review of gas explosion modelling.
4. To critically assess the strengths and weaknesses of available gas explosion models.
5. To recommend areas where further work is needed to improve the accuracy of the gas explosion models.

Scope

The following models were reviewed in some detail:

Name	Type	Grid	Discretisation accuracy	Reaction Model
TNT Equivalency	Empirical	N/A	N/A	None
TNO	Empirical	N/A	N/A	None
Multi Energy	Empirical	N/A	N/A	None
Baker-Strehlow	Empirical	N/A	N/A	None
Congestion Assessment Method	Empirical	N/A	N/A	None
Sedgwick Loss Assessment Method	Empirical	N/A	N/A	None
SCOPE	Phenomenological	N/A	N/A	Empirical Correlation
CLICHE	Phenomenological	N/A	N/A	Empirical Correlation
EXSIM	3D CFD Finite Volume	Structured, Cartesian, PDR Treatment of Sub-Grid Scale Objects	First Order Temporal Second Order Spatial	Eddy Break-Up
FLACS	3D CFD Finite Volume	Structured, Cartesian, PDR Treatment of Sub-Grid Scale Objects	First Order Reaction Progress Variable Second Order	Empirical Correlation
AutoReaGas	3D CFD Finite Volume	Structured, Cartesian, PDR Treatment of Sub-Grid Scale Objects	First Order Temporal and Spatial	Empirical Correlation
CFX-4	2D and 3D CFD Finite Volume	Structured, Body-fitted	Higher Order Temporal and Spatial	Eddy Break-Up and Thin Flame
COBRA	2D and 3D CFD Finite Volume	Unstructured, Cartesian, Cylindrical Polar or Hexahedral, Adaptive, PDR Treatment of Sub-Grid Scale Objects	Second Order Temporal and Spatial	Empirical Correlation
Imperial College Research Code	2D CFD Finite Volume	Unstructured, Adaptive	Implicit Temporal, Second order (TVD) Spatial	Laminar Flamelet and PDF Transport
NEWT	3D CFD Finite Volume	Unstructured, Adaptive	Higher Order Temporal and	Eddy Break-Up and Laminar

			Second Order Spatial	Flamelet
REACFLOW	2D and 3D CFD Finite Volume	Unstructured, Adaptive	First or Second Order Temporal and Spatial	Eddy Break-Up

Main findings

1. There is a wide range of class of models available - from empirical and phenomenological, through to those, which are CFD based. The latter category falls into two areas: 'simple' - many obstacles not resolved and 'advanced' - all obstacles resolved by the 3-D CFD grid.
2. Generally as one moves from empirical to advanced CFD, models become based on more fundamental physics, are able to more accurately represent the real geometry, but require increasing resource to set-up, run and interpret the results.
3. Models in each class embody a number of simplifications and assumptions, limiting their ability to be used as reliable predictive tools outside their range of validation against test data. It appears that only those models falling into 'advanced' CFD class could in principle be capable of being truly predictive tools outside their immediate range of validation. However, even here the existing models have limitations and require further development and testing before this capability is fully realised - which even then will currently be limited to relatively simple geometries by the required computer resources.
4. Many of the CFD-based explosion models in current use employ relatively crude approximations of the modelled geometry, relying on calibrated sub-grid models. In particular, the effects of those obstacles which cannot be resolved by explicitly by the CFD grid are often encompassed by applying a Porosity / Distributed Resistance (PDR) approach. This means that additional source and sink terms are added to the governing transport equations to mimic the effects of turbulence and momentum losses.
5. Most of the 'simple' CFD codes and some of the 'advanced' CFD codes most commonly used for explosion prediction use simple, dated numerical schemes for both the computational grid (often Cartesian only) and the finite differencing (often first-order), which could lead to substantial numerical errors. In addition, in practice the developers of the majority of PDR based CFD codes also recommend use of a single cell size. The codes are then compared and developed against experimental data for this size of cell. This effective calibration introduces an element of uncertainty: The codes may work well for scenarios that are similar to the calibration situation but in other instances the performance would be uncertain. Such a strategy does not guarantee grid independence of the final solution and, given the large recommended cell size, grid independence is unlikely. The end result is that these codes may be concealing large numerically generated errors.
6. The combustion models used in CFD-based approaches to predict the reaction rates are also subject to a considerable degree of uncertainty. In particular:
 - The eddy break-up combustion model, used by some of the 'simple' and 'advanced' CFD codes, requires a high grid resolution to yield a grid independent value of the burning velocity. The model also requires corrections to prevent unphysical behaviour near to surfaces and also at the flame leading edge to prevent numerical detonation. This has led most CFD explosion model developers to use empirical correlations for the flame speed, which are grid independent and implicitly include strain rate effects. Implementation of detailed chemical kinetics through the use of a PDF transport equation holds great promise for the future, but due to the heavy demand on computer resources in terms of both processor speed and computer memory, it is unlikely that this approach will be feasible for calculations of real complex geometries for perhaps another ten or more years.
 - There are large uncertainties with regards to rate data for many combustion related reactions; the combustion chemistry is extremely complex and may involve many tens of reactants and intermediate species in over one hundred reactions. It is possible to reduce the detailed kinetics

schemes to a smaller number of species (maybe only five or six species), but the resulting set of species conservation equations can become mathematically stiff, with the associated sensitivity to small changes in the dependent variables. Generally, explosion models represent the combustion reactions by a single reaction step involving fuel and oxidant species only. This simplification is necessary due to present constraints in terms of both computer memory and computer speed.

- Models which employ a prescribed reaction rate, could therefore be more sound than those relying on an Eddy Break-Up approach, because the latter requires a resolution of the flame front unlikely to be achieved in practice. Work is currently under way on the incorporation of detailed chemical kinetics into a gas explosion model, but it will not be feasible to use such a model on a real complex plant geometry in the foreseeable future. Thus a laminar flamelet combustion model has been implemented in the NEWT code. Qualitatively this model shows much better agreement with experiment than the eddy break-up model previously employed in NEWT.

7. The simple eddy-viscosity concept is ubiquitous amongst the explosion codes for modelling turbulent transport, but this model of turbulent transport is not strictly applicable in high speed, combusting flows, leading to further possible errors. There is a move to full Reynolds stress turbulence models, these have either been implemented in research type codes - currently not available on general release, or have not been tested for explosions. There are numerical stability problems associated with Reynolds stress transport models which need to be addressed.

The accuracy expected from, say phenomenological and 'simple' CFD models, is generally fairly good (to within a factor of two), e.g. the models yield solutions, which are approximately correct, but, importantly, only for a scenario for which the model parameters have been tuned. This limits the applicability of these models as truly predictive tools.

Main recommendations

1. There is a range of modelling approaches available, each with their own strengths and weaknesses. In order to establish greater confidence in model predictions, it is clear that, for the future, improvements in the physics and the numerics are required, particularly for the CFD-based approaches. However, predictive approaches are needed now. It is thus important that the user be aware of the uncertainties associated with the different models. The following recommendations are essentially those needed to be taken on board by model developers and their funders. They primarily relate to CFD models, which, in principle, should offer the best hope of becoming truly predictive models of gas explosions, with wide applicability.

2. Ideally one would replace the Cartesian grid / PDR based CFD models by models that are capable of representing a given geometry more accurately. However, the likely time scale for the necessary advances in computing power and code efficiency which will possibly allow geometries to be fully grid resolved is large, possibly of the order of ten years or more. Until this is possible a hybrid approach has to be adopted, whereby body-fitted grids are used to represent the larger objects within the explosion domain, with the PDR approach reserved for the regions that may not be resolved by the grid. It is therefore recommended that methodologies are developed to allow a seamless transition between resolved and PDR-represented solutions as grids are refined. There should be a move away from fixed grid cell size, because such models will require constant re-calibration for new scenarios due to physical and numerical errors associated with the large grid cell size always needing to be compensated. This situation cannot improve until there is a move to a more soundly based methodology.

3. More work is needed to establish the reliability of the combustion models used in CFD approaches. Presently, the majority of the explosion models investigated prescribes the reaction rate according to empirical correlations of the burning velocity. However, it should be recognised that these correlations are subject to a large uncertainty. The eddy break-up combustion model should ideally not be used if the flame front cannot be properly resolved or, the resulting errors should be recognised and quantified.

4. The sensitivity of model predictions to the turbulence model used should be investigated. Turbulence modelling has not yet received much attention in the field of explosion modelling. The commonly used two-equation, $k-\epsilon$ model has a number of known failings i.e. does not predict counter-gradient diffusion, but remains in use due to its economy and robustness. Large improvements in over-pressure prediction have been noted by including simple terms into the $k-\epsilon$ model, to account for compressibility effects. However, inclusion of these terms is by no means universal. There is a wide range of advanced, non-linear $k-\epsilon$ models now available. Ideally Reynolds stress transport modelling should be used but the models require much work to ensure that improvements are not offset by lack of numerical stability.
5. Model development should now be driven by repeatable, well-defined, detailed experiments, focusing on key aspects of the physics of explosions. This tends to imply small or medium-scale experiments. Large-scale experiments are suitable as benchmark tests, but code calibration on the basis of macroscopic property measurements should be treated with caution, since it is quite possible to obtain approximately correct answers but for the wrong reasons due to gross features swamping finer details. Detailed comparisons of flame speeds, species concentrations, etc., should allow deficiencies in explosion model physics and numeric to be identified, and solutions developed and tested.
6. There are no, or few, technical barriers to implementation of the above model improvements, beyond a willingness and need to do so.
7. Perhaps the safest that can be advised at this point is that it would be unwise to rely on the predictions of one model only, i.e. better to use a judicious combination of models of different types, especially if a model is being used outside its range of validation.

Reference

Ledin, H. S., 2002, "A review of the state of the art in gas explosion modelling", HSL report no. CM/00/04.

The views expressed in this article are those of the author alone, and should not be taken or inferred to be those of the UK Health & Safety Executive.

7. CASH FOR ARTICLES

Articles for the Newsletter, on any combustion-related topic, thoughts, activities or viewpoints, are always most welcome! In the case of full-time students registered at a UK university, the Combustion Physics Group Committee will award £50 for items accepted for publication. Articles should normally occupy between one and two pages in the Newsletter. Contact any of the Committee members (listed in Section 11) to discuss this topic

8. USEFUL WEBSITES

<http://www.iop.org>
<http://www.epsrc.ac.uk>
<http://monet.me.ic.ac.uk>
<http://www.cerfacs.fr/cfd>
<http://www.ge.com/aircraftengines/ge90>
http://www.gm.com/about/info/overview/RD_Center
<http://www.honda.co.jp/eng>
<http://www.lmm.jussieu.fr/Animations.html>
<http://www.forbrf.lth.se/spark>
<http://web1.mitsubishi-motors.co.jp/inter/technology/GDI>
<http://ivory.lm.com/%7Ecombus/index.html>
<http://cdr.stanford.edu/html/ME/faculty/mitchell.html>
<http://www.afrinc.com>
<http://www.itm.rwth-aachen.de/ercoftac/Welcome.html>

<http://www.ca.sandia.gov>
<http://www.et.byu.edu/cheme>
<http://www-mpl.sri.com:80/orgs/mpl.html>
<http://www.fe.doe.gov>
<http://www.altavista.digital.com>
<http://www.fetc.doe.gov>
<http://www.engin.brown.edu/faculty/suuberg>
http://vayu.che.caltech.edu/~ees/Faculty_overview.html
<http://www.lead.ruhr-uni-bochum.de>
<http://www.combustioninstitute.org>
<http://www.gk2k.ch.cam.ac.uk>
<http://www.opticspages.com/>
<http://www.zarm.uni-bremen.de/>

9. COMBUSTION DIARY

April 9-11, 2003: University of Cambridge, UK. Thermodynamics 2003, Thermodynamics and Statistical Mechanics with Industrial Applications . <http://www.the-conference.com/thermo2003/>

March 16-19, 2003: University of Illinois at Chicago. Third Joint US Section Meeting.
<http://www.cssci.org>

May 18-21, 2003: Jacksonville Florida, USA. 17th International Conference on Fluidized Bed Combustion. © Sarma Pisupati, Dept of Energy & Geo-Environmental Engrg, Pennsylvania State University, 110 Hosler Bldg., University park, PA 16802-5000. Phone: 1-814-865 0874; Fax: 1-814-863 5709; E-mail: fbc17@ems.psu.edu
<http://www.ems.psu.edu/egee/ShortCourses/FBC17.html>

May 22-23, 2003: Dessau, Saxony-Anhalt, Germany. 3rd Dessau Gas Engine Conference.
©Marianne Reppin, Phone: (49)34901 883 123; Fax:(40)34901 883 120; E-mail: dqmk@wtz.de

June 8-13, 2003: Marrakech, Morocco. Third Mediterranean Combustion Symposium. © F. Beretta, Italy, beretta@irc.na.cnr.it; N. Selcuk, Turkey: selcuk@metu.edu.tr; M. Mansour, Egypt, mansourm@aucegypt.edu.
<http://www.ichmt.org/Mcs-03>

July 7-10, 2003: Lisbon, Portugal. Clean Air 2003, Seventh International Conference on Energy for a Clean Environment. © Maria da Graca Carvalho, Instituto Superior Técnico - Mechanical Engineering Dept, Av Rovisco Pais, 1049-001 Lisbon, Portugal. Phone: 351-21 8417378; Fax: 351 21 8475545; E-mail cleanair@esoterica.pt
<http://navier.ist.uti.pt/cleanair/>

August 10-15, 2003: Ottawa, Canada. 39th IUPAC Congree and 86th Conference of the Cadian Society for Chemistry.
<http://www.nrc.ca/confserv/iupac2003>

September 18-21, 2003: Ischia, Napoli, Italy: Joint Meeting of the Scandinavian-Nordic and Italian Sections. © Associazione Sezione Italiana del Combustion Institute, c/o Dipartimento di Ingegneria Chimica, Università degli Studi di Napoli "Federico II".

secretary@combustioninstitute.it or Ass. Prof. Jens Klingmann, Dept of Heat & Power Engineering, Lund Institute of Technology, jens.klingmann@vok.lth.se. 100 Word abstract due April 30th, 2003 submit@combustioninstitute.it

October 18-21, 2003: First European Combustion Meeting sponsored by the Federation of the European Sections of The Combustion Institute. © Iskander Gökalp, CNRS - LCSR, 1C Ave de la Recherche Science, Orleans, France; Phone: (33)23 825 5463; Fax: (33)23 825 7875; E-mail: gokalp@cnrs-orleans.fr
<http://www.cnrs-orleans.fr/ECM2003/>

International Seminar on Fire and Explosion Hazards (8-12th September 2003) City Hotel Londonderry - www.engj.ulster.ac.uk/4thisfeh

MULTIPHASE FLOW 2003 Second International Conference on Computational Methods in Multiphase Flow

3 - 5 November 2003, Santa Fe, New Mexico
<http://www.wessex.ac.uk/conferences/2003/multiphase2003/1.html>

10. COMMITTEE MEMBERS CONTACT DETAILS

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