Engine Combustion Network: 2nd Workshop on Spray Combustion

Ignition and lift-off session

Contents: Page 1: Experimental work (Michele Bardi)
Page 2: Comparisons of models and experiments (Evatt Hawkes)

Experimental work

A summary of the experimental sub-session by coordinator Michele Bardi, CMT, mbardi@mot.upv.es
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LOL and ignition delay have been measured by the participating institutions at spray A conditions and for parametric variations about spray A.

Experimental setup

Time-averaged lift-off length: IFPEN, CMT, SNL agreed on the methodology using a narrow band-pass filter (310±5 nm) and an intensified camera. A long gate time was employed to obtain a time-averaged image (2 to 5ms ASOI for CMT and SNL, 0.8 to 1.3 for IFPEN). TU/e used a CMOS fast camera coupled with an intensifier (LaVision IRO) and a (310±5 nm) band-pass filter. The time-averaged image was obtained by the ensemble average of the images falling in the interval from 1.5 to 2 ms ASOI.

Ignition delay/time resolved LOL: CMT and SNL used broad band chemiluminescence imaging (CMOS camera, low pass filter <600 nm, with regular lens, 50 μs shutter time). IFPEN used the same setup with no filter. TU/e obtained ID and time-resolved LOL from the same experiment described the previous paragraph. Moreover TU/e tried an unfiltered test to improve the sensitivity to cool flames.

Results

LOL measurement: The time-averaged images were analyzed with the same processing method and a good consistency emerged between the facilities at spray A baseline conditions, (LOLsnl =17.2mm, LOLCMT =17.7mm, LOLTU/e =16.5mm, and IFPEN = 16.9mm). From the wide test matrix performed at CMT an empirical relationship has been developed to correct the bias that the real boundary conditions have from the boundary conditions. Moreover, the dependence on the outlet diameter from SAE 2005-01-3843 has been used to scale all the data to nozzle #677, the nozzle used by modelers. However the spread of the data remains similar: LOLsnl =17.46mm, LOLCMT =17.40mm, LOLTU/e =16.5mm, and IFPEN = 16.61mm.
The analysis of the time resolved LOL data showed that there are significant fluctuations of the LOL along the injection: the camera synchronization chosen has an impact on the results and likely explains the differences in the results observed.

The parametric variations tried showed good consistency between the different facilities. A higher increase in LOL in is observed for CMT and CAT (ECN1 data) when ambient temperature is reduced, but this difference is significant only below 800 K. This may be related to the presence of minor species in CVP or to some issue related to temperature boundary layer.

The selection of the threshold used for the LOL definition has a strong impact on the results and needs to be discussed when the LOL is computed at different test conditions. The suggestion is to scale the threshold for each test condition to the half of the intensity peak that is visible right after the LOL.

The comparison of the data obtained via broadband chemiluminescence data showed good consistency with OH* chemiluminescence data. However much care should be taken in avoiding background/liquid fuel reflection and saturation: all these factors contribute to modifying the intensity levels in the lift-off length region and thus reducing the accuracy of the measurements.

Cool-flames have not been detected by all the institutions due to different sensitivity of the camera and the different f/# of the lenses employed. The use of an intensifier (TU/e) without filter did not provide significant

improvements for the detection of cool-flames. However, combining the intensifier with the 310 band-pass filter allows precise detection of the second stage ignition. Even if the reference level of the cool flames could not be detected in all the cases, the sharpness of the intensity rise at the second stage ignition made the ignition delay measurement quite insensitive to the threshold adopted.

The values calculated by all the institutions are pretty close to 400 μs ASOI (IDsnl =400 μs, IDCMT =441 μs, IDTU/e =400 μs and IFPEN = 405 μs). The response to ambient temperature is pretty close for all the institution. Similarly to the LOL measurements, below 750K the ignition delay increases more for CMT rather than SNL, suggesting a consistent difference in the boundary conditions (temperature boundary layer / gas composition).

The comparison of pressure measurements from the CVP vessels showed consistency of the measurements with the data from chemiluminescence. The signal/noise ratio during the combustion is the most important issue of this technique: SNL showed that using an optimized setup it is possible to have a clear insight of cool flames and to distinguish them from second stage ignition under different test conditions (from 750 to 1200 K).

Comparisons of models and experiments

A summary of the modelling sub-session by coordinator Evatt R. Hawkes, The University of New South Wales, Sydney, Australia: evatt.hawkes@unsw.edu.au
17/11/2012

Scope

The session was focused on comparisons of models and experiments relating to lift-off length, ignition delay, and other available measures relating to gas-phase chemical reactions. Both n-heptane (spray H) and n-dodecane (spray A) were considered.

Objectives

The objectives were to compare different models against experiments for the purposes of validation and to identify what works and what needs improving, specifically in relation to issues of chemistry and turbulence-chemistry interactions.

Contributions

The following eight groups contributed modelling results:

- Argonne National Laboratory (ANL) – Sibendu Som, Douglas Longman
- ETH Zurich (ETH) – Michele Bolla, Yuri Wright, K. Boulouchos, G. Borghesi, E. Mastorakos
- IFP-Energies Nouvelles (IFPEN) – Julien Tillou, Christian Angelberger
- Pennsylvania State University (Penn. State) – S. Bhattacharjee, J. Jaishree, H. Zhang and Dan Haworth
- Politecnico di Milano (PoliMI) – Gianluca D'Errico, Tommaso Lucchini, Roberto Torelli
- Purdue University (Purdue) – John Abraham, Muhsin M. Ameen
- TU Eindhoven (TUe) - Sridhar Ayyapureddi,Ulaş Egüz,C. Bekdemir, L. M. T. Somers, L. P. H. de Goey
- University of New South Wales (UNSW) – Yuanjiang Pei, Evatt Hawkes, Sanghoon Kook

The contributions encompassed a range of different modelling approaches. Most of the contributions were RANS-based, and employed Lagrangian discrete phase models of the spray. An exception on both counts was IFPEN who contributed an LES model with an Eulerian approach to the spray. Several different approaches were used for modelling turbulence-chemistry interactions. A number of groups contributed well-mixed models, which ignore turbulent fluctuations of the thermochemical state. Compared with ECN1 there were more contributions using more sophisticated approaches. IFPEN, Purdue, and Tue contributed flamelet models, ETH contributed a Conditional Moment Closure (CMC) model, while UNSW and Penn. State contributed Transported Probability Density Function (TPDF) models.

The session was coordinated by Evatt Hawkes (UNSW), Michele Bardi (CMT), Christian Angelberger (IFPEN) and Yuanjiang Pei (UNSW).

Experimental/modelling comparison methods

A recommendation of ECN1 was to try to standardise and improve the methods for comparing experiments and models. Progress was made in this direction in ECN2, but differing definitions between modelling groups and between models and experiments still persisted.

Ignition delay

Experimentally, ignition delay was measured from the timing of sharp rises in chemiluminescence or pressure, which as discussed in the experimental part of the session, give consistent results. For the modelling, two definitions were recommended after ECN1:

1. First time at which Favre-average OH mass fraction reaches 2% of the maximum in the domain after a stable flame is established.
2. Time of maximum rate of rise of maximum temperature.

The definitions were compared using UNSW model results with two different models and agreed well. Five of the eight groups had used the recommended definitions in their contributed results.

Lift-off length

In the experimental session, it was recommended that lift-off should be measured using OH* chemiluminescence by finding the point of 50% rise of the chemluminescence to its peak value at the leading edge of the flame. After ECN1, it was recommended that the model definition should be given as the first location where ground state OH reaches 2% of its maximum in the domain. This definition proved controversial in ECN2 with many groups preferring locations which were further downstream.

UNSW implemented an OH* sub-mechanism in their model, and used a line-of sight integration of the OH* concentration in an attempt to obtain a surrogate for a chemiluminescence signal. Although the OH* sub-mechanism contains some known limitations, the results showed that OH* could have a very different profile to OH. The excited state showed a clear peak in the upstream region while the ground state levels increased monotonically downstream, owing to the presence of OH in the product gases. Thus it is not clear the extent to which OH can be used to determine lift-off in the models, and what OH threshold should be applied.

Analysis of UNSW's results for Spray A indicated that the lift-off predictions were significantly different between the different definitions adopted by the different groups, ranging from 17.5mm to 21.8mm. These differences were frequently as large as the differences between models and between models and experiment.

Model standardisation and boundary conditions

Chemistry models: For n-dodecane, it was recommended that the mechanism reported in [1] be adopted. For n-heptane, mechanisms reported at [2] and [3] were suggested. Amongst the contributions, there was a good convergence of chemical models for n-dodecane. For n-heptane the convergence was improved relative to ECN1 but there were still differences between the choices made by different groups.

Turbulence-chemistry interaction models: It was suggested that several groups could implement a well-mixed combustion model for comparison with the other models. Several groups did this, which resulted in some useful findings that will be discussed shortly.

Other: Standardisation of other elements such as spray models, numerical parameters such as grid, etc, was not attempted.

Comparison of experimental and modelling results

Conditions considered

- For Spray A, we considered a baseline ambient condition of 15% O_2, temperature 900 K, density 22.8 kg/m^3, with a 150 MPa injection pressure and 4 ms injection duration. We considered variations of temperature from 750 K to 1200 K and variations of oxygen from 13 to 21%.
- For Spray H, we considered a baseline of 21% O2, 1000 K, 14.8 kg/m^3, with 150 MPa injection pressure and long injection duration >4ms.

Overall remarks
Overall there was good agreement for qualitative trends for both ignition delay and lift-off length with some outliers. Most models over-predicted ignition delay and lift-off length for spray A while results straddled the experiments for spray H. The absolute agreement in both cases deteriorated with decreasing temperature and oxygen concentration. However, for ignition delay, relative errors remaining roughly constant across the temperature range considered.

Based on the contributions which were received, three questions were posed:

1. Do we get the same results with well-mixed models in different codes, etc?
2. Do flamelet and CMC methods give superior results compared with well-mixed models?
3. Do transported PDF methods give superior results compared with well-mixed models?

Do we get the same results with well-mixed models in different codes, etc?

For spray A, three groups had contributed well-mixed models and the chemistry models were also quite similar. Analysis of the results however indicated that despite the nominal similarities of the methods, we still obtained different results, which were the same order of magnitude as the differences between the different models and experiments. This indicates there is still a non-negligible influence of numerical errors or other peculiarities of the implementations.

Do flamelet and CMC methods give superior results compared with well-mixed models?

Several contributed results with flamelet-based methods were very good. However, the overall performance across the different groups and experiments considered was mixed. Comparison of the flamelet approaches with simpler well-mixed models was difficult because side-by-side runs were not done keep other factors held fixed.

The CMC results contributed by ETH showed greatly improved lift-off length and slightly improved ignition delay compared with a well-mixed model implemented by the same group.

Do transported PDF methods give superior results compared with well-mixed models?

UNSW found slightly improved ignition delay and greatly improved lift-off length with the PDF method for both Spray A and Spray H, and for both T_a and O_2 variations. Penn. State found greatly improved LOL and ignition delay for Spray A, but only slightly better ignition delay in spray H. (The chemistry model from spray H was more rudimentary.) Thus, PDF methods appear to improve results relative to well-mixed models. Of course, there is a significant trade-off for computational expense.

Summary of findings, discussion, and recommendations for future work

The participation was very good and everyone can be thanked for their contributions.

Definitions
Differing definitions are still a problem, particularly for the lift-off length. Since chemical sub-mechanisms for OH* are at a relatively early stage, it is generally not considered by modellers. Thus:

- It would be preferable if quantitative measurements of the ground state OH and/or other reacting scalars were available. Experience from the TNF workshop suggests that quantitative, simultaneous measurements of temperature and the major species needed to form a mixture fraction would be desirable.
- Further work is suggested to improve the kinetics of OH* and to incorporate OH* into the models.

Well-mixed combustion models
Well-mixed combustion models are attractive because they are computationally efficient and relatively straightforward to implement. The results show across the board that these models are capable of predicting basic trends. Further investigation of why this is the case seems warranted – is it that turbulent fluctuations are genuinely small or is it that the results are not sensitive to the fluctuations? They generally err on the side of over-predicting both ignition delay and lift-off length. This might be connected with the quite filamentary flames

that result in these models, which presumably lead to large rates of turbulent transport out of the reaction zone. Further analysis of the reasons for the observed trends would be useful.

It may be useful if a sub-set of the contributing groups try to converge on numerical parameters with their respective well-mixed models, in order to rule out numerical error as a reason for observed differences.

Flamelet combustion models
Relative to well-mixed models, flamelets can potentially improve modelling by improved treatment of fluctuations as characterised by non-trivial PDFs of mixture fraction, etc.. On the other hand they approximate chemistry by assuming that the thermochemical state space is very low dimensional and that it is the same as computed in a simplified counter-flow situation. Computationally, they are the most efficient of all the contributed approaches.

Although some very good results with flamelet approaches were reported, they were not consistent across the board and there was little useful information to enable a direct comparison with well-mixed models. More systematic investigations are recommended to determine the benefits and limitations of flamelet approaches.

CMC combustion models
CMC has similar advantages to flamelets with respect to treatment of fluctuations. CMC assumes the thermochemical state-space is locally one dimensional, but allows it to evolve in time and space. The results shown in ECN2 clearly show CMC is an improved model relative to a well mixed model. The computational expense is much larger, however.

TPDF combustion models
TPDF approaches have several advantages, notably treating the source term closure exactly and being quite general with respect to combustion regime. The results from ECN2 clearly show the TPDF model is an improved model compared with the well-mixed model. This comes with a price of significantly larger computational expense however, suggesting avenues to reduce the cost of this method should be investigated.

Suggested future modelling targets

ECN3 would benefit by continuing to pursue the existing target cases. Much has been learned compared with ECN1, but several issues remain outstanding and further investigation is required.

Additional target cases could consider

- Multiple injections: The situation of a single, high momentum injection is relatively straightforward for RANS. LES practitioners might be more interested in having more transient situations such as might arise in multiple injections. In addition, multiple injections might result in a more demanding test of turbulence-chemistry interaction models since the injection of new cold fuel into an already burning and mixing environment might result in different combustion behaviours.
- Larger nozzle: Those interested in heavy duty applications might be interested in a larger fuel nozzle. This could result in the regions of spray and combustion overlapping, which might result in a more demanding test of models and the need to consider spray-combustion interactions with a greater level of detail.
- Walls: With industry trends towards longer lift-off lengths, the wall is becoming increasingly important. Scenarios such as re-entrainment or heat loss at the wall might result in different combustion behaviours which models cannot yet capture.

[1] Sarathy, Mehl, Westbrook, Pitz, Togbe, Dagaut, Wang, Oehlschlaeger, Niemann, Seshadri, Veloo, Ji, Egolfopoulos, Lu, Comprehensive chemical kinetic modeling of the oxidation of 2-methylalkanes from c7 to c20, Combustion and Flame 158(12), 2011, pp. 2338–2357, Mani.Sarathy@kaust.edu.sa
[2] Lu et al. 53 species: http://www.engr.uconn.edu/~tlu/mechs/mechs.htm
[3] Seiser et al.
https://www-pls.llnl.gov/?url=science_and_technology-chemistry-combustion-nc7h16_reduced_mechanism