First International Workshop of the Engine Combustion Network, ECN1

Summary

Experimental and modeling activity under the Engine Combustion Network has expanded significantly over the last several years. In an effort to coordinate future research related to engine spray combustion, the ECN met for its first workshop. ECN1 was held the 13-14 May 2011 in Ventura, California, several days prior to the ILASS 2011 Conference. 53 participants from 14 countries attended the workshop, while 16 more accessed the live presentations via webcast.

The workshop addressed experimental and modeling activities at two conditions that have received significant attention: the “Spray A” and “baseline n-heptane” conditions. Multiple laboratories have prepared their facilities to operate at Spray A conditions and have completed characterization measurements of the spray. In addition, over 10 different groups have performed CFD simulations of Spray A and baseline n-heptane conditions. Organizers gathered experimental and modeling results at these conditions and provided side-by-side comparison at the workshop, including a summary and recommendations for future practices.

Experimentally, the control of boundary conditions at high-temperature, high-pressure ambient and injector conditions (Spray A and others) is non-trivial. This workshop served as an exchange platform to discuss techniques for controlling boundary conditions. Researchers that have already established control of boundary conditions assisted those that are preparing their facilities.

While improvement of CFD models by direct comparison with experimentation is a primary goal of the ECN, comparison of models and experiments is hindered by experimental and modeling uncertainties. These uncertainties include, for example, the measurement of spray boundary conditions, such as rate of injection, as well as those downstream of the nozzle exit. Progress will be made when these uncertainties are minimized. After exchanges between experimentalists and modelers on these subjects, recommendations were given for best experimental methods to (1) standardize experiments and (2) provide the most quantitative information. Common modeling approaches and evaluation criteria were also chosen.

The workshop was divided into two major sections, with focus on experimental and numerical approaches in diesel sprays. A summary of findings, conclusions, and recommendations for future work are given in each section, followed by the presentations given at the workshop. Proceedings from ECN1 are available to download from the website.

IMPORTANT NOTE ON USE OF THIS MATERIAL

Results of the ECN Workshop proceedings are contributed in the spirit of open scientific collaboration. Some results represent completed work, while others are from work in progress. Readers should keep this in mind when reviewing these materials. It is inappropriate to quote or reference specific results from these proceedings without first checking with the individual author(s) for permission and for the latest information on results and references.

ECN1 Workshop Final Program

<u>Friday- 13 May 2011</u>

8:00am Registration & Continental Breakfast	
9:00am Introduction & Mechanics	Lyle Pickett, Sandia National Labs
9:20am Spray A Experimental Efforts	Gilles Bruneaux, IFPEN
9:50am *Vessel Temperature*	Maarten Meijer, Eindhoven
10:15am *Ambient Composition*	Jaclyn Nesbitt, MTU
10:40am *Nozzle and injector temperature*	L.M. Malbec, IFPEN
11:05am *Nozzle geometry*	Alan Kastengren, Argonne
11:35am Break- Lunch provided	
1:30pm Spray A Experimental Efforts continued	
1:30pm *Hydraulic characterization*	Raul Payri, CMT
1:55pm *Liquid Length*	Caroline Genzale, GaTech
2:20pm *Vapor penetration*	Tim Bazyn, Caterpiller
2:45pm *Combustion*	Lyle Pickett, Sandia
3:10pm Discussion	
3:45pm Break- light snack provided	
4:15pm Spray A Computational Efforts	Sibendu Som, Argonne
Argonne	Sibendu Som
UW-Madison	Chris Rutland
Poly Milano	Gianluca D'Errico
Sandia	Lyle Pickett
UNSW	Yuanjiang Pei
5:10pm Spray A Computational Effort Results	Sibendu Som, Argonne

<u>Saturday- 14 May 2011</u>

8:00am Registration- beverages provided only	
8:30am Baseline n-heptane Experimental Efforts	Lyle Pickett, Sandia
8:50am Baseline n-heptane Computational Efforts	Evatt Hawkes, UNSW
Cambridge	Giulio Borghesi
CMT	
Eindhoven	Bart Somers
UW-Madison	Chris Rutland
Penn St	Dan Haworth
9:30am Break- snack and refreshments provided	
10:00am Baseline n-heptane Computational Results	Evatt Hawkes, UNSW
10:50am Discussion	
11:30am Future Directions	
Spray B, 3-hole Diesel Injector	
Gasoline Direct Injection	
Canonical Engine Flows	Sebastian Kaiser
Modeling & Experimental Working Groups	
Next Workshop	
1:00pm Break- Lunch provided	
3:00pm Discussion- Droplet Breakup Theory on San Buenaventura State Beach	

Summary of presentations and discussions

Session leaders for experimental and computational work have written a summary abstract of their sessions below. Full presentations are found in links on the website.

Ambient Gas Temperature

Group Leader: Maarten Meijer (Eindhoven University of Technology – TU\e)

Contributors: Louis-Marie Malbec and Gilles Bruneaux (IFPEN), Lyle Pickett (Sandia National Laboratories), Raul Payri, Michele Bardi, Julien Manin (CMT), Tim Bazyn, Glen Martin (Caterpillar)

Summary of the Ambient Gas Temperature Measurements Working Group Session

Aim of the session is to provide guidelines for ECN spray A ambient gas temperature characterization. Guidelines are provided for hardware implementation and post processing methods. 2 different set-ups can be distinguished; pre-burn combustion vessels and constant flow rigs. Both type of set-ups are capable to reach spray A conditions. The fundamental difference in the operation of both set-ups lead to different measurement approaches to characterize the ambient temperature field.

For the constant flow test rigs time averaged measurements are executed both at Caterpillar and CMT. Based on the followed measurement approach, conventional hardware; thermocouples, signal conditioners and DAQ, can be selected. Different thermocouple diameters (at the same position) are used at both institutes in order to define the required radiation correction. Corrections are based on extrapolation to 0 [mm] diameter. The ambient temperature is measured at different locations inside the flow rigs. Ambient gas temperature fluctuations of +/- 10 [K] are reported based on 10 [s] and 20 [s] averaged measurement data for Caterpillar and CMT test rigs respectively. Wall temperatures are 800 [K] found at both facilities. No information on measurement deviations and error bounds is provided at this moment.

Temperature characterization for the pre-burn combustion vessels is executed at Sandia National Laboratory, IFPEN and TU\e. The wide temperature range which is crossed as a result of the used precombustion method in combination with the small time scales lead to an unconventional (thermocouple) measurement approach. Main goal of the executed measurements is to define the relation between the vessel core temperature and the bulk temperature. The bulk temperature is measured by using a piëzo-electric pressure sensor. All 3 institutes used fine wire thermocouples to define the core temperature. The used thermocouples are capable to follow the fast temperature change inside the combustion vessel. Sandia and TU\e implemented an adjustable probe with 5 different 50 [μm] thermocouples. The Platinum material from the type R thermocouples can result in an undesired catalytic respond when installed in the sequentially filled type pre-burn combustion vessels (used at IFPEN and TU\e). Therefore IFPEN used a 25 [μm] thick, single K-type thermocouple. At TU\e a Nitrogen/Oxygen mixture was used (no filling of pure oxygen), to avoid this undesired effect. High speed DAQ hardware is selected in combination with high measurement accuracy as well (number of bits). Signal conditioners can be used but direct logging of the [mV] signal from the thermocouples is also possible, applying cold junction and linearization afterwards. A similar approach is followed by all 3 institutes to correct the measured thermocouple signal for radiation and the convective respond. At the spray A injection temperature (900 [K]), the influence of these corrections is small. Measurement deviations at spray A are around 10 [K]. Measurement uncertainties are believed to be +- 7.5 [K], but are still under investigation. The found relation for the core and bulk temperature is 1.03 for IFP and 1.08 for Sandia and TU\e. Measurements with the type-R thermocouple probe show high temperatures at the top of the combustion vessel, caused by buoyancy effects.

References: Comparison of diesel spray combustion in different high-temperature, high-pressure facilities. L.M. Pickett, C.L. Genzale, G. Bruneaux, L-M Malbec, L. Hermant, C. Christiansen, J. Schramm. SAE 2010-01-2106

Engine Combustion Network: implementation and analysis of combustion vessel spray A conditions M.Meijer, R.J. Christians, J.G.H. v. Griensven, L.M.T. Somers, L.P.H. de Goey Illass-Americas 23rd conference paper number 151

Discussion Issues & Future Investigation

Constant flow: Until now, only time averaged ambient gas temperature measurements are executed. It seems that temperature fluctuations are small but the fluctuations over time are not investigated. This can be relevant for the temperature error estimation. Fine wire thermocouples are required for this.

Pre-burn combustion vessels: Further characterization of the temperature field right before fuel injection is required because small temperature fluctuations have a profound impact on ignition delay, spray penetration and the flame lift off length. Especially the temperature field close the fuel injector should be investigated and analyzed more in detail. More investigations on the used TC corrections (for radiation, convective respond and conduction) are ongoing which are critical in order to define the reached measurement uncertainty.

Ambient Composition Session

Group Leader: Jaclyn Nesbitt (Michigan Technological University - MTU)
Contributors: Maarten Meijer (Eindhoven University of Technology), Louis-Marie Malbec and Gilles Bruneaux (IFPEN), Lyle Pickett (Sandia National Laboratory), Raul Payri (CMT), Tim Bazyn (Caterpillar)

Summary of the Ambient Composition Working Group Session

The focus of the ambient composition working group for the ECN1 Workshop was to examine the different methods of creating the thermodynamic state for the charge gas in experimental apparatuses including combustion vessels and constant pressure flow rigs in the Engine Combustion Network (ECN) under the ‘Spray A’ test condition. This was accomplished by comparing the different institutions ambient compositions and modeling their impact on autoignition of n-heptane as a diesel fuel surrogate. The slides presented at the workshop are provided, and a brief overview of the comparisons made with the key results outlined here.

First, the four preburn combustion vessels (Sandia, MTU, IFPEN, and Eindhoven) were compared in regards to preburn mixtures used which consist of varying levels of C_2H_2, C_2H_4, H_2, O_2, N_2 and Ar. This comparison was accomplished using a single-zone chemical kinetics model in Cantera interfaced with Matlab with the GRI 3.0 mechanism to compare minor species produced during the preburn and levels at injection. The different cool-down temperature histories of the vessels (heat transfer modeled as convective with a temperature trace being a quadratic exponential decay) were also modeled. The peak preburn temperature of Eindhoven is largest, followed by MTU, Sandia, and IFP. Although MTU and Sandia utilize the same preburn mixture, MTU uses a fan speed seven times that of Sandia which results in a higher peak temperature and a faster rate of cool down. MTU and IFP have similar cool-down rates, with Sandia having the longest cool-down time due to the low fan speed used. These differences (premixed gas mixture and cool-down rate) cause variations in minor species, NO is largest for Eindhoven, followed by MTU, Sandia and IFP due to the temperature trends from the preburn, but in all cases the levels at the time of diesel injection are more than 50 times less than equilibrium levels, with similar trends for NO_2. For OH, this species tracks the temperature-time trace and at injection IFP has the maximum OH (attributed to the largest level of H2 in the preburn mixture), followed by Eindhoven, MTU and Sandia, with these levels being one to two orders of magnitude less than equilibrium values. At equilibrium, for IFP NO in 3030 ppm and OH is 170 ppm, for MTU and Sandia NO is 5100 ppm and OH is 230 ppm, and for Eindhoven NO is 5250 ppm and OH is 240 ppm.

Additionally, for the conditions at injection the four preburn vessels major species (CO_2, H_2O, Ar, N_2, and O_2) were compared to the CMT and Caterpillar constant pressure flow rigs which use O_2 and N_2 to achieve the desired 15 percent oxygen conditions for 'Spray A'. Comparison included the major species levels and constant pressure specific heat capacities. Finally, the stoichiometric n-heptane ignition delay was determined using chemical kinetics modeling with a reduced mechanism to compare the influence of ambient compositions major species levels and the different minor species produced during the preburn on autoignition, relative to that of dry air and air plus ideal residuals to simulate EGR. Results showed that the preburn vessels, despite their respective differences in minor species at injection, did not significantly impact the ignition delay of n-heptane. More specifically, the vessel ignition delays were 4% shorter than ideal EGR and 83% longer than dry air. Comparing the preburn and constant pressure vessels major species at fuel injection, the specific heat capacities are similar (spanning 1.13 to 1.21 kJ/kg-K at 900 K), and the variation in ignition delay is within the modeling accuracy. More specifically, when considering major species only, IFP had the shortest ignition delay (0.65 ms), followed by CMT / Caterpillar at 0.69 ms, and the remaining preburn vessels of 0.72 ms. Again, the ignition delay was longer than that of dry air as expected due to the reduction in oxygen level at the 'Spray A' condition. There are however noticeable differences in the peak temperature of n-heptane ignition between the different vessels with the Nitrogen / Oxygen constant pressure flow rigs having a peak temperature at 45 K higher than the preburn vessels. Key conclusions are that despite the differences in preburn mixtures and ambient compositions, the ambient charge-gas compositions for the vessels considered show no significant differences in fuel ignition delay at the condition considered or mixture constant pressure specific heat capacity.

Also discussed briefly was a recent *Energy and Fuels* journal publication with a goal of isolating and understanding chemical kinetics effects on the preburn process and autoignition of n-heptane fuel while including minor species and neglecting spray dynamics. The key conclusions can be found in the slides, with the main result being that the combustion vessel with the preburn procedure is an effective tool for studying spray combustion over a range of ambient conditions without concern over the reactive minor species produced by the preburn procedure. The citation is listed below for reference for further review.

Nesbitt, J.E., Johnson, S.E., Pickett, L.M., Siebers, D.L., Lee, S-Y., Naber, J.D., 'Minor Species Production from Lean Premixed Combustion and Their Impact on Autoignition of Diesel Surrogates,' *Energy and Fuels* 25 (3), pp. 926-936, 2011.

Discussion Issues & Questions

The key observation and conclusion from the above and the workshop is that there is no significant effect of ambient composition differences on the specific heat and autoignition delay of n-heptane as a diesel surrogate. There are however noticeable differences in the flame temperatures and the consequences of this are unknown. Further unknown is the potential differences in ignition or combustion duration as a result of these ambient environments. Questions were brought up on if the time-step used in the model influences the results (a consistent time-step was used in all of the modeling, however, there was no sensitivity study undertaken), the influence of other n-heptane stoichiometries in addition to the lambda one case studied here, and if the n-heptane mechanism used influences the results. These questions are continuously being addressed with additional modeling work.

Recommendations & Future Investigation

It is recommended that experimental testing is undertaken to characterize the differences in ambient gas composition between the vessels in regards to major and minor species levels and autoignition delay of the fuel. MTU has conducted some exhaust gas sampling, however this sampling was not in-situ, not in real-time in the vessel, nor under 'Spray-A' conditions. Sandia has tried some measurements of the exhaust gases but found that there are large levels of unburnt hydrocarbons due to the large amount of crevice volumes in the CV (think of the CV as a cube with 6 pistons (access ports) as the crevice volumes). Sampling directly in the CV is difficult but is something that would be useful experimentally and to also validate this simplified chemical kinetics preburn modeling.

The modeling used in this work involved a simplified single-zone model, and using a more detailed two-cell or multi-cell model would improve the accuracy and applicability of the modeling simulations. LLNL expressed some interest in looking into this, but this will be extremely complex to the differing vessel geometries.

Spray A Nozzle Tip Temperature Measurements

Louis-Marie Malbec, IFPEn
Contributors:
Lyle M. Pickett – Sandia National Laboratories
Raul Payri, Julien Manin, Michele Bardi – CMT Motores Térmicos
Tim Bazyn, Glen Martin – Caterpillar
Maarten Meijer, L.M.T. Somers, Technische Universiteit Eindhoven
Alan Kastengren, Argonne National Laboratories

Summary of the workshop session:

This session presented Spray A nozzle tip temperature measurements conducted at 6 contributing institutions: Sandia, IFPEn, CMT, Caterpillar, TUE and Argonne.

As an introduction, the fact that it is impossible to measure the fuel right at the outlet of the injector was reminded. The measurement techniques and results shown in this presentation were thus attempts to access this fuel temperature as close as possible, through the measurement of the nozzle body temperature.

The first part of the presentation described the different devices used by the contributing institutions, with an emphasis on the impact of the characteristics of the vessels on the fuel temperature:

- For continuous flow vessels (CMT, CAT) or cold flow vessels (Argonne), the vessel walls and ambient gas temperature are constant, so the injector is in steady state (no temporal evolution of its temperature).
- For preburn vessel, the ambient gas temperature is increasing during the combustion and then decreasing during the cool down process. The temperature of the injector and of the fuel is thus changing with time.

Besides, continuous flow vessels and preburn vessel require cooling systems to control the injector (in the cold flow vessel, the injector is heated). The geometry of these cooling systems and their ability to limit the heat rise may have an effect on the fuel temperature.

At last, a ceramic cover is used to protect the nozzle tip from the ambient gas hot temperatures, and thus also to limit the temperature rise of the fuel.

In the second part, the three different techniques used by the institutions to measure the nozzle tip temperature were presented.

The first one consists in putting a thermocouple on the injector’s body, quite far from the nozzle tip. This type of measurement is relevant when the injector is in steady state and has been performed by CMT an Argonne.

The second one, carried out at IFPEn, is based on the Laser Induced Phosphorescence (LIP), which allows the measurement of the temperature of the surface of the nozzle tip, and its evolution during the preburn event.

The last one requires the use of a dummy injector equipped with a K-type thermocouple. This technique allows the measurement of the temperature within the sac volume, and gives access to its temporal and spatial evolution. At the moment of the workshop, only Sandia, TUE and CAT have used this dummy injector.

In the third part, of the presentation, the results were analyzed.

The temperature measured in the sac volume with the dummy injector is first compared between Sandia and TUE. This comparison shown great differences both in the amplitude of the temperature rise during the preburn, and of its evolution during the cool down event. But it is difficult to know whether these differences are due to variations in the efficiency of the ceramic shields, in the efficiency of the cooling systems or in the cool down behaviors. So no conclusion was drawn so far.

The effect of the ceramic shield has also been investigated by IFPEn (LIP) and TUE (dummy injector). The results shown similar temperature evolutions, however at different levels, for theses two institutions, in spite of the different techniques used. The temperature of the surface of the nozzle tip seems thus to be strongly correlated with the sac volume temperature. Moreover, the ceramic shield used by TUE seems to be slightly more efficient than IFPEn, as the temperature rise is higher at IFPEn.

At last, the use of the dummy injector also allowed assessing the temperature gradients within the injector (Sandia, TUE, CAT). This showed a slight decrease of the temperature when the distance to the sac volume increases, but no conclusion can be drawn concerning the effect of such a gradient on the injected fuel temperature.

As a conclusion, the difficulty to correlate the different temperature measurements with the real temperature of the injected fuel and its evolution was underlined.

Recommendations:

- In order to assess and control the temperature of the injected fuel, the temperature must be measured in the sac volume.
- The dummy injector technique is the best one to access the sac volume temperature because of its simplicity (the post treatment is also quite easy) and of its accuracy.
- The use of a ceramic shield is a good way to limit the temperature rise of the sac volume. The design of TUE one's seems to be the more efficient.
- When using a cooling system, people must be careful of the corrosion that can be induced by water condensation on the injector tip.

Discussion items from the workshop:

- As an answer to a question on the effect of the fuel temperature on liquid length, it was reminded that this was of first order, and thus needs to be controlled as precisely as possible.
- The modelers underlined that for the moment, there was no model able to take into account the heat transfers between the fuel and the injector's body within the nozzle hole. Thus, the temperature of the injected fuel right at the outlet of the injector can not be inferred from its temperature in the sac volume.

Nozzle Geometry and Needle Motion Session

Group Leader: Alan Kastengren (Argonne National Laboratory)
Contributors: Christopher Powell (Argonne National Laboratory), Lyle Pickett and Peter Lillo (Sandia National Laboratories), Raul Payri and Julien Manin (CMT), Tim Bazyn (Caterpillar)

Experimental Techniques

It is well-known that the detailed nozzle geometry in spray nozzles can profoundly impact the spray behavior. To better understand the ECN spray behavior, four different measurement techniques have been used to measure the nozzle geometry. Caterpillar has performed static x-ray tomography with a laboratory x-ray source. Argonne has performed phase-contrast imaging of nozzles using a synchrotron undulator source. Sandia has performed optical and SEM microscopy of the nozzle exit region. Finally, CMT has performed silicone molding to characterize the internal geometry. Argonne has also performed time-resolved phase-contrast x-ray imaging of the injector needle motion to characterize the three-dimensional motion of the needle during the injection event.

Findings

- X-ray tomography measurements provide the best base dataset for the nozzle geometry, as the data are quantitative, three-dimensional, and cover the entire nozzle tip region.
- X-ray tomography results suffer from some artifacts and drawbacks, which can be corrected using the other measurement techniques.
    - The spatial resolution of the tomographic reconstructions (3 μm transverse, 8 μm axially) is insufficient to precisely define the nozzle exit diameter.
    - Tomographic reconstruction shows oscillations in the nozzle wall that are not seen in the phase-contrast images.
- Optical microscopy provides the best measure of the nozzle exit shape and size.

- SEM looking into the nozzle hole provides perhaps the only feasible non-destructive method to determine the nozzle surface roughness, but requires dismounting the nozzle from the injector.
- Silicone molding has the best potential to determine the nozzle inlet diameter, but requires dismounting the nozzle from the injector.
- Nozzle K-factors vary, but tend to be around 2 – 2.5. The exit diameter of all nozzles seems to be less than 90 µm, which has important implications regarding the determination of nozzle flow coefficients.
- Tomography and phase-contrast imaging both show a significant narrowing of the nozzles for about 50 µm near the nozzle exit. This seems consistent for the various nozzles.
- The needle motion for each injector is highly repeatable from injection to injection. The needle motion is complex and three-dimensional, with significant oscillatory off-axis motions.
- The axial needle motions are quite similar between all injectors tested. The lateral motions of the needle are unique to each injector.

Recommendations & Future Investigation

- There is a lack of cross comparisons between the different techniques to measure nozzle geometry. Efforts are ongoing to complete a more comprehensive set of measurements with each of the techniques.
- Given the significant asymmetries seen in the nozzle geometry, all ECN experimenters should carefully record the injector orientation for their measurements. The recommended reference is the injector fuel inlet (which also aligns with the flats on the injector).
- A consistent methodology must be developed to create a reference geometry (preferably in STL format) for use in CFD modeling of internal nozzle flow.

ECN Workshop 1 - Hydraulic Characterization

Group Leader: Raul Payri (CMT – Motores Termicos - UPV)
Contributors: Julien Manin and Raul Payri (CMT), Lyle Pickett (Sandia National Laboratories), Tim Bazyn (Caterpillar) and Alan Kastengren (Argonne National Laboratory)

Summary of the Hydraulic Characterization Working Group Session

The hydraulic characterization group has two main objectives: first to provide accurate data to the community concerning rate of injection, spray momentum and hydraulic coefficient; and second, to compare the measurements between facilities and estimate the eventual difference between injectors. The first part explained the difference related to the measurement of the mass flow, Sandia and CMT both provided data in this respect, using two different approaches: the Bosch "long tube" method for CMT and the mass adjusted rate of momentum for Sandia. Higher oscillations have been observed and analyzed for the long tube method when compared to the ROI measured by Sandia. The analysis showed that the oscillations were generated by an axial translation of the injector thus compressing the testing fluid section of the rate meter, which has been correlated with needle motion measured at Argonne. The momentum flux has been measured by CMT, Sandia and CAT. Both CAT and CMT have the sensor placed orthogonally to the spray while the spray hits the sensor at a 30^o angle in Sandia's facilities. The measurements showed good agreement between facilities and injectors except for 210678 that presents higher rate of momentum. An analysis of the oscillations recorded by the pressure transducer placed on the feeding line demonstrated the influence of the length of this line, but more interestingly, it has been observed that the amplitude of the fluctuations was related to the injection system upstream (e.g. high-pressure pump, lines and regulation device). Finally, a complete analysis of the measurements has been carried out by changing injection and discharge pressures to hydraulically characterize the injectors through C_d, C_a, C_v as well as the effective velocity and diameter.

Conclusions

The conclusions drawn for the hydraulic characterization session were that pretty good agreement between research institutes as well as similarities in the way of measuring these parameters. One concern has been pointed out though, injector 210678 showed higher rate of momentum according to CAT compared to the other injectors of the set. The vibration analysis performed to understand where the oscillations on ROI came from revealed that the fluctuations on ROI and momentum signals were similar and related to a displacement of the needle and injector. If no experiment is possible and since all the nozzles in the ECN are (should be) very similar, the best way to obtain the injected mass and spray momentum can be achieved using the dimensionless coefficients (C_d, C_v, C_a) that should be close for all nozzles (210678?). If a difference in diameter is observed, it has been seen to affect strongly the discharge coefficient C_d and the area coefficient C_a but not to influence the velocity coefficient C_v, this must be affected by an injection pressure problem though. To obtain mass flow rate from spray force measurement the following formula should be applied before adjusting the injected mass:

$$\dot{m}_f \propto \sqrt{\dot{M}_f}$$

Discussions

The first comment made after this session was the lack of data concerning direct measurement of the injection rate as it does not require expensive installation, only CMT directly measure the ROI and Sandia measured it indirectly. The Bosch “long tube” method proved not to be appropriate to generate an exact rate of injection for modelers due to the high oscillations present on the signal. Injector 210678 must be sent to Sandia for further analysis of the possible higher spray momentum (compared to other injectors of the same family). Spray momentum measured at CMT and CAT showed similar features and pointed out a possible sensor resonance at Sandia. There is a need for experimentalists to provide accurate injection rate signal to modelers as this is the starting point of the process and the impact on later results is huge. Raul Payri (CMT) said he would discuss about generating a “virual” injection rate with the other members of the injection group when back in Valencia.

Experimental uncertainties

When it comes to hydraulic characterization, the errors or uncertainties on the experimental side come from different sources. When talking about uncertainties, a difference shall be made in this case between precision and accuracy of the experiments. Starting with the precision, mounting the injector several times in the test rigs (either flow rate meter or spray momentum facility) may lead to slightly different results. Specific analysis has been carried out to address this and showed that the maximum deviation was about 1% (corresponding to spray momentum, this value for injection rate is about 0.6%), which is in agreement with previous studies performed at CMT. Concerning the accuracy of the experiments, care must be taken to what kind of measurements we are looking at. For instance, rate of injection when measured by the Bosch “long tube” method presents large oscillations, which have been analyzed and are now known to be an artifact of the experimental technique. The transient regions cannot be taken as recorded and displayed; either for momentum or mass flow rate, signal filtering and experimental arrangement may shift the signals away from the reality of the physical process. Finally, the maximum uncertainty of the measurement for the steady period (value) of the injection has been estimated to be below 4% for both experimental techniques.

Recommendations and bottom line

The first recommendation concerning the hydraulic characterization is that every injector should be tested as some differences have been seen within this set of "identical" injectors. The hydraulic characterization is a necessary step for the experimentalists as it provides important data to the modelers and slight variations may induce important differences in mixing and combustion. Care must be taken when performing hydraulic characterization, because although injection rate and spray momentum are two essential parameters, they require expertise to be carried out correctly. Additional efforts are needed in this field as the diagnostics are not able to provide precise and accurate enough data for model predictions. The design of a "best guess" for the injection rate has been taken by CMT (Dr. Jaime Gimeno is working on a "virtual" injection rate) and should be discussed by the ECN participants before releasing the information.

Spray A Liquid Length Measurements

Caroline L. Genzale, Georgia Institute of Technology

Contributors:

Lyle M. Pickett, Caroline L. Genzale – Sandia National Laboratories
Gilles Bruneaux, Louis-Marie Malbec – IFPen
Raul Payri, Julien Manin, Michele Bardi – CMT Motores Térmicos
Tim Bayzen, Glen Martin – Caterpillar

Summary of the workshop session:

This session presented Spray A liquid length measurements conducted at 4 contributing institutions: Sandia, IFPEn, CMT, and Caterpillar.

Each institution conducted liquid length measurements by Mie-scatter imaging, an easily implemented liquid-phase detection technique commonly used by the diesel and gasoline spray research communities. An initial comparison of the Mie-scatter measurements at each institution revealed that the reported liquid lengths at the Spray A condition spanned approximately 3 mm: 8.2 mm (CAT), 10.6 mm (Sandia), 10.8 mm (CMT) and 11 mm (IFPen). Noting that this is a fairly substantial range, the session was primarily focused on discussing the potential reasons for such a variation in measured liquid length between the contributing institutions.

In the first portion of the presentation, one potential source of dispersion in the liquid length measurements was discussed: lack of consistency in the Mie-scatter experimental setup at each institution. An overview of the experimental setups revealed that each institution featured a unique combination of illumination source, direction and scattered light detection. A review of recent work at Sandia was presented to demonstrate the influence of these experimental variables on the quantified liquid length when performing Mie-scatter imaging. They applied a variety of illumination and imaging setups to Spray A. They found that the liquid length could be quantified up to 2 mm longer than their reported value of 10.6 mm by saturating the scattered light signal. They also found an increase of about 1 mm when the spray is illuminated from the head-on direction rather than from the side. These shifts in the quantified liquid length occur because the axial location and intensity of the peak scattering signal can change based on the illumination intensity, direction and scattered-light collection. Thus, when assigning a threshold or relative intensity cut-off to define the liquid length (typically 3% of the maximum signal), the axial location of that cut-off is dependent on the axial location and intensity of the measured peak scattering signal (which is dependent on the experimental setup). It was demonstrated that a scale factor can be applied to the data to bring the relative intensity behavior of the different experimental setups in line, but such a scale factor would be generally unknown.

The session also briefly discussed another potential source of dispersion in the liquid length measurements: facility-to-facility variations in ambient and/or fuel temperature. It was noted that based on work presented in the previous sessions, there may be differences in operating temperature at the 4 facilities. For example, IFP set their injector coolant temperature to achieve a nozzle temperature of 60°C prior to their premixed burn, while Sandia operated with a nozzle set-temperature of 90°C prior to the premixed burn. Liquid length predictions based on the Siebers mixing-controlled vaporization model were presented, showing that this 30°C difference can contribute to liquid lengths that are approximately 1 mm longer at IFP than at Sandia, consistent with a reported longer liquid length at IFP. Payri et al. (CMT) demonstrated a similar sensitivity to fuel temperature experimentally. Variations in ambient temperature are also expected to influence liquid length, but facility-to-facility variations in ambient temperature where not as readily apparent.

In the last portion of the presentation, a discussion ensued on alternative liquid length measurement techniques, based on light extinction. In addition to the collection of Mie-scatter techniques applied to Spray A, Sandia also applied two different light extinction measurement techniques: line-of-sight laser extinction along the axis of the spray and diffuse back-illumination imaging. As discussed during the session, these techniques may be preferred over Mie-scatter imaging because light extinction measurements are essentially self-calibrating. That is, they are based on direct measurement of an intensity ratio (I/I_o) and yield a measurement of optical thickness based on Beer's Law. Based on this premise, it was suggested that the use of an optical thickness measurement to define the liquid length might provide a less ambiguous metric for facility-to-facility comparison over the use of a relative Mie-scattering intensity, which is based on a peak signal that is sensitive to experimental setup. In addition, it was demonstrated that these techniques pose the promise of quantifying liquid volume fraction and/or droplet sizes since the measured optical thickness is dependent on these quantities. However, it was also shown that diffuse back-illumination imaging can be influenced by beam steering by the clipping of light rays at the collection aperture, yielding uncertainties in the measured optical thickness and making the lowest levels of optical thickness undetectable.

Discussion items from the workshop:

- Based on the difficulties presented in unifying Mie-scatter liquid length measurements, the group generally agreed that a light-extinction technique should be considered for recommendation as the standard ECN liquid-length measurement technique.
- A key consideration expressed by many members of the ECN was the importance of selecting a liquid length measurement technique that could be easily implemented at each of the facilities.
- It was also pointed out that consistency between the measurements is likely to be of more importance for this task than quantitative accuracy. The primary goal of these measurements is to verify that each facility has reached the Spray A condition, not necessarily to provide a quantitative measure of liquid length for model validation

- Though beam steering present in the back-illuminated extinction images may contribute to uncertainty about the precise location of liquid length, the group believed that a comparison of the extinction drop-off behavior just upstream of the liquid length could provide a more robust comparative measure than Mie-scatter imaging.

Recommendations:

- The standard liquid length measurement to verify the Spray A condition should be performed using diffuse back-illumination at 532 nm (green LED).
- A comparative measure should be defined in order to assess the consistency of the measurement at each institution. A strict threshold based on optical thickness may not be appropriate since beam steering prevents detection of the lowest optical thickness levels near the spray tip. The optical thickness "drop-off" just upstream of the spray tip offers a potential metric. This metric should be assessed once several contributing institutions have completed back-illumination measurements of Spray A.
- The influence of beam steering on the measured optical thickness should be assessed.
- Groups wanting to use this data for validation of CFD models should be made aware of the limitations of this measurement data for use as a quantitative measure of the liquid length. A further assessment of beam steering effects on the measured optical thickness and the potential to measure low levels of optical thickness near the spray tip is needed.
- A rigorous methodology for setting fuel delivery temperature is necessary to eliminate this source of facility-to-facility variation in the liquid length.

Evaporating and Combusting Vapor Penetration Session

Group Leader: Tim Bazyn (Caterpillar Inc.)
Contributors: Louis-Marie Malbec and Gilles Bruneaux (IFPEN), Lyle Pickett and Caroline Genzale (Sandia National Laboratory), Raul Payri, Jean-Guillaume Nerva, and Julien Manin (CMT), Tim Bazyn and Glen Martin (Caterpillar)

Summary of the Vapor Penetration Session

The focus of the vapor penetration working group for the ECN1 Workshop was to examine the methods and results for measuring the penetration of the evaporating or reacting fuel spray at the Spray A conditions.

Vapor Penetration, the distance from the nozzle to the leading edge of the fuel spray, is one of the fundamental measurements that has historically been used to quantify spray jets. It has been selected as one of the primary measurements for Spray A, meaning that spray penetration should be verified at spray A conditions before performing additional measurements. It is an easily observable and quantifiable phenomenon that is robust to experimental and processing methodology and it measures an important parameter in engine spray and combustion performance that provides an indicator of the mixing and spray processes.

The primary methods for measuring vapor penetration are shadowgraph and schlieren-based techniques, which measure the bending of light through the test section (2nd or 1st derivative of the index of refraction, respectively). These techniques use the same basic components – light source, large collimating and collecting optics, imaging lens, optional schlieren stop, and camera. Some variation in setups among the contributing institutions include chromatic and/or pulsed light sources, which can aid in rejection of combustion luminosity, and schlieren stop, with Caterpillar and Sandia using no stop, IFP using a disc for a dark-field schlieren arrangement, and CMT using an aperture for a bright-field schlieren arrangement. All the contributing institutions used an image processing routine developed at Sandia that looks at the texture of the temporal derivative of the series of images to define the spray region. Thus, the processing technique works best when measurable signals are achieved everywhere in the spray image, and saturated or dark regions are avoided. Additional processing is performed to smooth the edges, fill the holes, and add regions to the spray definition that were excluded because they were either very luminous or obscuring. This process involves sensitivity settings that must be matched to the optical set-up, currently in an ad hoc matching of the measured spray region with the apparent spray region. The maximum penetration of this spray region is reported as spray penetration.

Comparisons of the techniques showed that a properly set-up focused shadowgraph technique was sensitive enough to capture the edge regions of the spray, and that the additional sensitivity of a Schlieren set-up was not desired because it typically enhances the dark or bright regions that should be avoided. Also, temporal or chromatic filtering with a pulsed or monochromatic light source was preferred to eliminate combustion luminosity to avoid saturated regions for the same reason.

The sensitivity of cone angle and penetration was discussed, based on a discussion from Pickett et al. (SAE 2011-01-0686). While penetration measurements are relatively insensitive to optical set-up, cone angle measurements show a pretty significant sensitivity to optical setup and processing parameters. Comparisons with Rayleigh scattering measurements and the non-uniform mixing model of Musculus and Kattke (SAE 2009-01-1355) indicate that a high-sensitivity shadowgraph set-up captures the cone angle that corresponds to near zero fuel concentration. From this discussion, penetration will continue to be the primary measurement of bulk spray behavior due to its insensitivity to experimental method. However, future discussion of ECN contributors should address the addition of cone angle data to the ECN to capitalize on all the information that is available from spray shape measurements.

A review of the current results from ECN participants showed relatively good agreement among the groups. The data generally showed an agreement between the non-reacting and reacting cases up to the point of ignition, after which the combusting sprays showed an increase in penetration due to gas expansion from heat release. A few of the observed discrepancies were discussed:

- IFP observed earlier deviation between non-reacting and reacting conditions, explained by an earlier ignition delay due to higher ambient temperatures.
- CMT showed faster penetration after 2.5 ms after the start of injection due to a longer injection duration for their experiments, which was examined and verified with experiments of different duration at Caterpillar.
- Caterpillar observed slightly slower penetrations, which was explained as possibly a difference in the discharge coefficient or spreading angle, which agrees with spreading angle measurements which showed wider sprays. This is potentially explained by hotter orifice temperatures leading to changing flow conditions such as cavitation.

Data on the sensitivity of the spray penetration to density and injection pressure was also presented. This data provides some parameter sensitivity for model validation, one of the items mentioned in the discussion. Also, relatively good agreement was observed between Caterpillar and Sandia measurements for injection pressure sensitivity.

Summary of Experimental Uncertainty

Each institution provided an experimental uncertainty estimate, and this estimate is displayed in the slides on the graphs as light colored bands. The primary source of uncertainty is shot-to-shot variation. Each institution completed 5-12 repeats of the Spray A measurements leading to an uncertainty of the mean penetration length of 2-3%. Additional sources of uncertainty include optical resolution, nozzle position, and nonlinearity, but these sources represent less than 1% uncertainty. The variation in experimental conditions also creates some uncertainty in how accurately the experiments represent spray A conditions, and these values are provided in the presentation showing that most institutions matched spray A conditions within 1-2%.

Discussion Issues & Questions

The recommendations of vapor penetration methodology were agreed upon with little discussion. Discussion followed on the use of cone angle measurements in the ECN. The general thought was that experimental parameters would need to be standardized to enable cone angle measurement reporting, although consensus was not reached on how to do this. It was also discussed that additional sensitivity to key parameters should be measured to enable the correction of experimental data that deviates from the nominal condition as well as for model validation of parameter sensitivity.

Recommendations & Future Investigation

The recommendations for future ECN vapor penetration methodology were:

- Focused shadowgraph technique with high sensitivity
- Avoid bright, saturated flame regions (if possible) with chromatic or temporal filtering
- Use the available Sandia-developed processing algorithm of the texture of the temporal derivative as the spray indicator
- Define penetration as the maximum penetration of spray region
- Conduct future experiments with quantitative mixture fraction results to determine how this definition corresponds to mixture fraction
- Develop standardized experimental methods and processing algorithms for additional spray shape information that is available from data, such as cone angle

Spray A Combustion Session

Group Leader: Lyle M. Pickett (Sandia National Laboratories).
Contributors: Tim Bazyn and Glen C. Martin (Caterpillar), Louis-Marie Malbec, Laurent Hermant, Gilles Bruneaux (IFPEN), Michele Bardi, Julien Manin, and Raúl Payri (CMT), Lyle M. Pickett and Caroline L. Genzale (Sandia National Laboratories)

Experimental Approaches

The processes that drive ignition and combustion for Spray A include all of those discussed previously, including careful gas and fuel temperature control as well as the vaporization, mixing, and penetration. However, ignition and lift-off length are expected to have a very high sensitivity to temperature (exponential). Combustion experiments are therefore expected to provide increased scrutiny about the similarity in operation between different facilities.

Direct luminosity imaging using high-speed cameras is the preferred method for ignition detection, at least for second-stage high-temperature ignition. Imaging of 310-nm emission using intensified cameras for detection of OH* chemiluminescence is the preferred technique for lift-off length measurement, although high-speed imaging at other wavelengths is also possible. Schlieren imaging can also be used to detect cool-flame and high-temperature ignition (SAE 2010-01-2106). The table below summarizes the approaches used to date at various institutions for Spray A.

	type	*injector*	*310 nm transient*	*310 nm time-ave*	*<450 nm*	*<600 nm*	*Natural unfilt.*	*Schlieren*
IFPEN	preburn	676	few	X			X	
Sandia	preburn	677	few	X	X	X		X
CAT	flow	677/678		X	X	X		X
CMT	flow	675	X	X			X	

Light imaging is the most straightforward option for comparison between facilities because flow-type vessels do not have controlled pressure rise from which to extract heat-release rate. The pressure rise from closed-volume, preburn-type vessels may be analyzed with respect to simultaneous light imaging, but care must be taken to account for small levels of heat release and speed of sound correction for the pressure wave. Preburn vessels also have residual CO2 and H2O, presenting compositional differences compared to flow vessels diluted with only N2.

Findings

- Luminosity imaging is sufficient for detection of ignition using non-intensified high-speed cameras, but exposure times greater than about 50 μs are necessary (and full-open lenses). Short-wave-pass filtering is recommended after ignition, because of the intense soot luminosity.
- Luminosity imaging with sensitivity for soot luminosity (1-5 μs, low f/#) does not have dynamic range to measure first high-temperature chemiluminescence.
- Schlieren imaging shows appearance of a cool-flame (first stage-ignition) at approximately 250 μs ASI. No measurement of cool-flame chemiluminescence was attempted.
- High-temperature (second-stage ignition) occurs at approximately 400 μs ASI at Caterpillar and Sandia, with an uncertainty of approximately 50 μs based on the camera framing period. Luminosity imaging for ignition at IFPEN and CMT was inconclusive because of limited camera sensitivity. However, indications are that ignition delay was slightly shorter at IFPEN and higher, at CMT.
- After correction for time delay based on the ignition location and the pressure transducer, the measured pressure rise correlates well with the luminosity increase. This measured pressure rise provides further information about heat release not attainable in open flow vessels.
- Time-averaged profiles of 310-nm emission show a "leveling-off" or "knee" followed by a decline of intensity with increasing axial distance. The decline is not as sharp at higher wavelength (<450 nm).
- Using the "leveling-off" as a threshold to define quasi-steady lift-off length, the order in lift-off length follows a similar trend between institutions as ignition delay. Where shorter ignition delays are measured, the lift-off length is less. The mean lift-off length value between institutions is approximately 17 mm, with variation of about ±1.5 mm. This difference is more significant than the statistical uncertainty at any institution, and likely indicates systematic temperature differences.
- No trends with respect to ignition or lift-off length could be associated with preburn vs flow vessels, suggesting that minor species or inert major species are not as significant as other variables.
- When ambient temperature is intentionally varied, and lift-off length is analyzed in the same way, the measured lift-off lengths over a range of temperature are in good agreement between institutions, including both preburn or flow vessels.

Overall, these results show that comparable combustion data can be generated in different types of combustion vessels. Combustion results perhaps even show less variation between facilities than spray liquid length, for example. Ultimately this suggests that Spray A datasets between flow vessels and preburn vessels can be linked, and future research may be leveraged.

Recommendations & Future Investigation

The recommendations for future ECN combustion methodology are:

- Use the measured "leveling-off" high-temperature chemiluminescence (imaging line-of-sight) as a reference. Use 50% of this value as a threshold when defining ignition delay and lift-off length. This luminosity intensity reference is orders of magnitude higher than cool-flame chemiluminescence and orders of magnitude weaker than soot luminosity, but it must be determined for the specific imaging arrangement. The reference can be measured for Spray A with sufficient sensitivity by permitting soot luminosity to saturate the imaging system after high-temperature ignition.

- For specific conditions, perhaps not at Spray A, determine the leveling-off value and base lift-off length upon this value. Further research is needed to determine how the leveling-off value depends upon wavelength.
- Use two high-speed pressure transducers of different gain settings in constant-volume chambers, with the high-gain transducer reset shortly before ignition to provide a sensitive measurement of ignition and pressure rise due to the spray.
- Use LIF of formaldehyde and OH to more precisely define first- and second-stage ignition. Couple these measurements to high-speed luminosity and schlieren imaging for greater understanding of routine high-speed diagnostics.
- For modeling purposes, axial profiles of ground-state OH may be used to define lift-off length. However, future models should incorporate emission from excited electronic-state OH, including chemical reactions that include OH* emission for a better match to the experiment.
- Moving beyond the Spray A temperature of 900 K, let ambient temperature be a part of future parametric studies. For example, Spray A-800 K, Spray A-950 K, and so forth. Post recommended temperature targets on the ECN website.

ECN Workshop 1 – Spray A Modeling

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Gianluca D'Errico*, Tommaso Lucchini, Daniele Ettore (Politechnico di Milano - Polimi),
Lyle Pickett* (Sandia National Laboratory - Sandia),
Yuanjian Pei*, Evatt Hawkes, Shawn Kook (University of New South Wales - UNSW)

Summary of Spray A modeling session

The primary objective of the Spray A modeling session was for different modelers to use their best practices in matching the spray A non-reacting data. The non-reacting data used for validation included liquid spray penetration vs. time, vapor penetration vs. time, mixture fraction vs. radial position at a given time, location of vapor and liquid boundaries at different times. Four different codes were used namely: CONVERGE (ANL), KIVA-3V (UW), OpenFOAM (Polimi) and FLUENT (UNSW). In addition, 1D correlations developed at Sandia were also used to predict vapor penetration and mixture fraction distribution. The group leaders of each modeling group gave short presentation of their modeling approach and grid size used. All the simulation approaches adopted the Lagrangian approach for the discrete phase modeling.

The group coordinator then summarized all results from different research groups. Parametric studies were performed to quantify the influence of grid size, time-step size, and turbulence models on liquid and vapor penetration vs. time. It should be noted that the definition of liquid length and vapor penetration was different for various modeling approaches. Different turbulence models tested included RANS (standard k-ε, Realizable k-ε, and RNG k-ε) and LES models (such as Smagorinsky and dynamic viscosity). Further, in order to facilitate apples-to-apples comparison, simulations with same minimum grid size, similar time-step size, models, and model constants were performed with CONVERGE, OpenFOAM, and FLUENT.

Conclusions

1) Liquid penetration: Quasi-steady liquid length was well predicted within 3-4% accuracy by all the models despite differences in modeling approaches and definitions. Liquid spray boundaries were well captured by ANL and Polimi models. However, initial transience was not well captured by any of the modeling approaches.
2) Vapor penetration: Vapor penetration was fairly well captured by all the simulations, UNSW probably doing the best job. In addition, ANL and Polimi were able to capture the location of vapor boundaries very well at 0.5 and 1ms. However, at 1.5ms vapor penetration is underpredicted, consequently, spray dispersion is overpredicted.
3) Mixture fraction distribution: Sandia correlations and modeling results from ANL and Polimi captured the Gaussian mixture fraction trends well. At certain instants though the predictions were beyond the experimental error bars.
4) Effect of grid size: Simulation results are not grid independent for the grid size range studied. Spray and vapor penetration increase with decrease in grid size for the RANS models.
5) Effect of time-step size: Liquid and vapor penetration results from ANL were time-step independent. Vapor penetration results from Polimi were time-step independent, however, liquid spray penetration results were not.
6) Effect of turbulence model: Turbulence models had pronounced effects on vapor penetration while effect on liquid spray penetration was negligible. Best vapor penetration results were predicted by the RNG k-ε model using CONVERGE and realizable k-ε model using OpenFOAM. Dynamic viscosity based LES results from UW for spray penetration seemed to be grid independent. Increased flow structures are observed with smaller grid sizes using LES models from both UW and ANL.
7) Despite differences in models, grids, and modeling approaches different best practice approaches were able to capture experimental trends fairly well, which is not surprising. Next set of simulations were performed with same minimum grid size, similar time-step size, models, and model constants. Liquid and vapor penetration results revealed significant differences between ANL, Polimi, and UNSW simulations. The reasons for these differences warrant further investigations.

Discussion and Recommendations

1) Liquid penetration: Liquid length fluctuations can be reduced by injecting higher number of computational parcels. Initial transience can be better reproduced with an accurate ROI, accounting for the nozzle flow and needle lift effects, accurate discharge coefficient values. Influence of spray model constants on this initial transience also needs to be characterized. Spray breakup model constants perhaps have the most significant influence on spray penetration.
2) Vapor penetration: Modelers need to focus on the early and late parts of vapor penetration profiles where discrepancy with experimental data is the largest. This may improve the spray dispersion predictions also.
3) Mixture fraction distribution: This is a difficult parameter to match. Future studies should focus on matching the mixture fraction decay along the centerline also.
4) Full 3-D simulations will be more accurate than 2-D simulations.
5) Location of modeled injector exit in mesh should be stated by modelers (e.g. are drops inject from the center of a cell or from a cell vertex?).
6) LES models need to be improved for matching vapor penetration and distribution.
7) Minimum grid size should be refined to 0.125mm to observe if grid independence on parameters like liquid and vapor penetration.

Future work

1) The major outcome of this session was to ensure that the next set of simulations are presented with standardized definitions of parameters like liquid and vapor penetration. Please refer to the summary sheet for the n-heptane baseline modeling session on recommendations for these definitions.
2) Spray A data was under one well-defined operating condition. Since all these models have tunable constants, matching data at one operating point is not very difficult. Parameters such as ambient temperature, injection pressure etc., need to be varied to characterize its influence on liquid and vapor penetration values. Such data will provide a more rigorous test-bed for different modeling approaches.
3) Future simulations from different groups need to employ same models, model constants, Schmidt number value, n.o. parcels injected, initial turbulence levels, grid size, time-step size etc.
4) Validation against combustion parameters such as lift-off length and ignition delay could not be performed in the absence of a reduced chemical kinetic mechanism. The session coordinator is collaborating with Lawrence Livermore National Laboratory and University of Connecticut to develop an appropriate reduced chemical kinetic mechanism for dodecane combustion. The aim is to develop a reduced mechanism consisting of 100 species or lesser for simulations.

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Model comparisons: baseline n-heptane condition

(A summary by the session coordinator Evatt R. Hawkes, The University of New South Wales, Sydney, Australia: evatt.hawkes@unsw.edu.au)

Summary of contributions

The session compared models and experiments of non-reacting and reacting n-heptane sprays performed in the Sandia constant volume chamber.

The following nine groups from five different countries contributed modeled data:

- Argonne National Laboratory: Sibendu Som, Douglas Longman
- Cambridge University: Giulio Borghesi, Epanimondas Mastorakos
- Universitat Politècnica de València CMT: Ricardo Novella, José Pastor, Francisco Payri, J.M. Desantes
- TU Eindhoven: Bart Somers, Cemil Bekdemir, L.P.H. de Goey
- Penn. State: Dan Haworth, Hedan Zhang, Subhasish Bhattacharjee
- Politecnico di Milano: Gianluca D'Errico, Tommaso Lucchini, Daniele Ettorre
- Purdue: John Abraham, Chetan Bajaj
- UNSW: Yuanjiang Pei, Sanghoon Kook, Evatt Hawkes

- U. Wisconsin ERC: Yue Wang, Gokul Viswanathan, Rolf Reitz, Chris Rutland

A wide range of models was considered. Most groups were using RANS while one group contributed LES results. Most of the spray models were based on the Lagrangian discrete phase approach, though one work contributed an Eulerian approach, while another contributed a “gas-jet” model. There were few common threads among the choices of spray sub-models, with different groups choosing to adopt a different set of models. Similarly, in the reacting cases, a number of different chemical kinetic models were featured. Turbulence-chemistry interaction models had more consistency, with most contributors choosing a well-mixed model, exceptions being one conditional moment closure model, one unsteady flamelet progress-variable model, and one partially stirred reactor approach.

Non-reacting comparisons

Liquid length

Inspection of the definitions used revealed that nearly every group had adopted a different definition for the liquid length. Most were based on the position at which a certain percentage of the total liquid fuel mass in the domain could be found between that position and the nozzle, however the actual numbers chosen varied somewhat.

Despite the different definitions, most of the models could reasonably match the experimental steady-state liquid length. This was presumably due to the model coefficients being adjusted to achieve a match. This underlines a need for parametric studies in the experiments to ensure that models can respond appropriately to parametric changes.

The transient period of liquid injection was less consistent but as this period is shorter than the typical ignition delays, it might not be too critical for the prediction of reacting cases.

Vapor penetration

Similarly to case of the liquid length, it was shown that nearly every group adopted a different definition for vapor penetration. Most were based on a threshold of fuel mass-fraction, but again the numbers chosen were not consistent. An analysis of the experimental data showed that if the threshold fuel mass-fraction was chosen to be sufficiently small, it should provide a reasonable agreement with the experimental results based on a threshold applied to schlieren images.

Most of the models predicted the vapor penetration reasonably well. Some slightly under-predicted the penetration, but at least one of these results is probably due to the well-known round-jet anomaly of the standard k-epsilon model. The reasonable agreement obtained highlights the need for parametric studies in order to better expose what is not working rather to simply demonstrate that the models can work with tuning.

Mixture fraction

Mixture fraction thankfully has an unambiguous definition, which facilitates comparison of the models. Comparisons were made at the axial distances of 20 and 40 mm at a time of 6ms after start of injection, as well as the results at the axial station 17mm at 0.49ms. Although there were some outliers in the mixture fraction results, the comparisons were good for the majority of the models. More differences were found closer to the nozzle and at the earlier time. It was not clear what caused the differences between models, but is speculated that some of these differences might be due to grid convergence or statistical convergence, and different assumptions regarding the rate of injection (the measurement of which has experimental uncertainties).

Reacting comparisons

Lift-off Length

The lift-off length (LOL) was also defined differently by different groups. Some were temperature-based and some were OH mass-fraction based.

The compilation of 13 different results for the variation of the LOL with the ambient O_2 percentage showed that all of the models were able to predict the qualitative trends but that many of the quantitative predictions were not good. A selection of four models that performed quantitatively very well revealed that there was no common element such as the chemistry or the turbulence-chemistry interaction sub-models. Therefore a clear conclusion cannot be drawn at this stage.

The fewer results for lift-off length trends with temperature that were contributed showed better agreement that the trends with O_2 fraction, while the only contribution with different ambient densities simply showed that the trend was qualitatively predicted, but not quantitatively.

Some groups had contributed data with the same chemical kinetic sub-models. Comparison of these revealed that even if the same chemistry and turbulence-chemistry interaction model were chosen, the results were still different between groups. There does however appear to be a benefit in going to more detailed chemical kinetic models, with good results being demonstrated by a 52 species n-heptane mechanism due to Lu et al. [1] and a 159 species skeletal mechanism due to Seiser et al. [2].

Ignition Delay

The definitions of ignition delay varied even more widely than those of the previous parameters, with most being temperature-based.

Overall, similar trends were observed in the ignition delay and the lift-off length in terms of whether the trends could be captured by at least some of the models. However, closer inspection revealed that some models which had captured the lift-off length well could not capture the ignition delay, and vice-versa. This potentially indicates that different mechanisms might be at play in controlling the two parameters.

OH fields

Although there was no experimental data to compare with, several modeling groups contributed some planar slices showing OH mass-fraction. These were quite revealing since, despite the predicted lift-off lengths being quite similar, the actual OH fields showed strong structural differences between the models.

Particularly noteworthy was the comparison of the well-mixed models with a CMC model. The well-mixed models feature an extremely and unrealistically thin OH layer at the leading edge that is very difficult to resolve. (Other minor species are actually even worse than this.) These thin structures may result in high mixing rates of radicals from the flame, which might affect or possibly even control the stabilization. It is not clear whether this dissipation of radicals at the large scale would be in any way comparable to the true dissipation which actually happens on much smaller scales. In contrast, the CMC model, which allows turbulent fluctuations of mixture-fraction, shows a much broader and smoother profile that seems physically more realistic.

Discussion and Recommendations

Definitions

The session highlighted the need for consistent definitions between the modeling groups in order to make meaningful comparisons.

The following were the results of the discussion:

- Liquid length would be better defined as a local liquid volume fraction. A level of 0.15% was suggested. An alternative definition would be simulated extinction. It was suggested that an experimentalist could volunteer to provide an algorithm for determining this.
- For vapor penetration, it was agreed that a threshold of mixture-fraction was a good definition and a value equal to 0.001 was chosen.
- For lift-off length, it was agreed an OH mass-fraction was a sensible definition, and value of 0.00025 was suggested.
- For ignition delay, there was no consensus. The experimental definition based on pressure might not be appropriate for those who are not simulating the actual chamber geometry. It was suggested that several definitions be tried and compared.

Spray models

It was clear that, having seen the experimental data, we are mostly able to predict the spray behavior with the models by varying the empirical constants used in those models. In order to learn how to improve the models, an experimental parametric study might be a lot more useful than just having one case. Blind tests might be useful to avoid extensive parameter tuning.

Another suggestion was to agree on a set of sub-models to use for the spray to see if their implementations in different codes resulted in large differences of results. However there was little support for this suggestion.

Chemistry and turbulence-chemistry interaction models

It was suggested that, in order to remove the complexity of spray modeling and let some groups focus on turbulence-chemistry interactions, one group who was obtaining good results for the spray behavior might provide a set of boundary conditions after the liquid length for the gas-phase part of the problem. However, it was noted that the possibility that the spray might be existing in supercritical conditions would appear to invalidate all of the spray models being used, leaving a means of how to provide this boundary condition uncertain.

It was suggested that in order to focus on differences between the models for turbulence-chemistry interaction, that small number of chemical kinetic sub-models could be chosen and used by the whole group. It was agreed that the previously mentioned [1] and [2] were good targets, but it was also noted the large size and the stiffness of the latter mechanism may present computational expediency issues for some models.

Summary and recommendations

- The participation was very good and everyone can be thanked for their contributions.
- The results mainly showed that trends could be captured but still there are quantitative differences. Due to the large number of things varied between the models and the way results were reported, it was difficult to draw any clear conclusion yet about what is working and what is not.
- One of the glaring inconsistencies was of the definitions. It is recommended that consistent definitions should be adopted by all of the modeling groups. The draft set outlined above are a good starting point.
- There is limited opportunity to make progress in spray modeling with only one case available and many empirical constants to adjust. Advances in predictive spray modeling will probably require a wider parametric range to be studied experimentally.
- Using a consistent chemical mechanism between different groups may be beneficial to focus on other aspects. Two chemical mechanisms were suggested and generally agreed upon.

Future Directions

This session was dedicated to discussions about future orientations of the ECN. Different topics were discussed concerning experimental and modelling directions as well as the organisation of the next ECN workshop.

At first, the topic of canonical engine flows was introduced by Sebastian Kaiser, motivated by the need to extend the database realized within the ECN towards more realistic engine database. The Sandia hydrogen engine database available on the ECN website was taken as an example. The difficulties related to the extension of the ECN Spray A database to engine type database was discussed. It was decided to form a working group on this topic led by Sebastian Kaiser, with the objective of drawing a road map on this subject.

Then the subject of parametric variation around Spray A conditions was discussed. Different parameters of interest were mentioned and it was decided that guidelines should be provided by the ECN to specify common parameter variations. Among the parameters of interest, temperature appears to a first order one. Injection pressure, injection duration and oxygen concentration were also mentioned. It was decided to name those parametric variation as Spray A followed by the changed parameter value (for example: Spray A 950K, Spray A 750K, spray A 1000bar...). Also the interest of measurements at spray B conditions (3 hole Diesel injector) was discussed.

The subject of the modelling work group was then discussed. A work group had been active before the workshop on the experimental side but not on the modelling side. It was decided to form a modelling workgroup led by Evatt Hawkes and consisting of the institutions that participated to the modelling sessions of ECN1 (Spray A Computational Effort Results and

Baseline n-heptane Experimental Efforts). The objective of this workgroup will be to coordinate modelling efforts and to provide guidelines on the comparison between modelling results. Also it was decided that the use of the ECN webpage would be discussed in the next modelling webmeeting. It was decided to organise separate experimental and modelling meetings within the next four month and a joint experimental/modelling meeting in 8 month to exchange on the conclusions of each working group.

The next topic was Gasoline Direct Injection. Different issues where discussed. In particular the subject of injector technology was highlighted. The choice of single or multi-hole injectors was discussed. 2 hole injectors seem to have the advantage of presenting a good compromise between simplified and representative geometry since the effect of jet to jet interaction seems to be a key issue. It was decided to form a work group on this topic led by Scott Parish.

Finally the organisation of the next ECN workshop, ECN2, was discussed. It was decided to hold the next workshop approximately 18 month after ECN1 and in Europe. An interesting possibility would to organize ECN2 jointly with ICLASS (September 2-6, 2012 in Heidelberg, Germany) since the synergy was ILASS was proven to be fruitful. It was decided to contact the ICLASS chairman to investigate this possibility. Other possibilities were proposed (ECN2 joint with LES4ICE or with Thiesel).

Discussion- Droplet Break-up Theory on San Buenaventura State Beach

The last session of ECN1 was the most important. All the participants joined the San Buenaventura State Beach. An experimental investigation of the secondary break-up of wave droplet clouds was carried out using almost non-intrusive boogie board sensors. However because of the high uncertainties of the measurements it was not possible to conclude on the thermodynamical pathway of the wave, the possibility that wave break-up might be occurring at supercritical state is still open, especially when considering the high tube roll up pressure increase induced by the wave break down... Then, in order to investigate the origin of primary wave break-up, a remote study of the wind motion was carried out using volley ball sensors. However again the experimental campaign was not successful due to the high uncertainty on the position of the field borders, especially when French guys were around... It all ended by a unfruitful but pleasant discussion about completely different subjects... Therefore it was decided that this session should absolutely be renewed in the next workshop to finally try to come up with a conclusion!

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