**Minutes of ECN 8 Diesel Topics**

**Topic 1: Internal flow and near-field**

Michele Battistoni, University of Perugia.

The objective of this topic was to ***investigate the internal flow and near-nozzle region, up to ~10 mm, with focus on fuel effects, by comparing n-dodecane vs. OME.*** Published guidelines made up a call for contributions on experiments and simulations with both dodecane and OME3. Four institutions provided new data, mainly simulations, with comparisons of fuels on spray C and D. Two institutions also included spray A. Novel experimental data regarding OME-3 is lacking, only hydraulic characterization was received from one institution. One submission was on jet breakup simulation, but still with limited resolution compared to the actual needs for diesel sprays.

The analyses focused on the sprays steady state behaviors and on fuel effects.

MAIN RESULTS:

* Investigating fuel effects is not trivial. Despite variations are not large, the impact can be important on the spray, mainly in the external spray.
* The internal nozzle behavior seems very similar between the two fluids. Cavitation in spray C is predicted to have the same structure with OME-3 as with n-dodecane.
* Hydraulics data indicates that mass flow rates scale quite well with the square root of the density ratio, as expected theoretically.
* The external jet and spreading are more affected by the fuel properties. A unanimous consensus has not been reached. However, it seems that OME-3, having slower jet velocities under the same injection pressure, tends to produce a longer intact core. Models however should better address these aspects.
* OME-3 properties need to be better assessed. In particular, the specific heat seems to be somewhat controversial, even if in the near nozzle topic, it has a marginal effect.
* Transient effects have not been studied with OME-3: an area for future investigations.
* Cone angles and plume growth need to be validated against specific data, which are currently missing for OME3.

ADDITIONAL COMMENTS:

* Knowledge of transition from near nozzle to spray in hot conditions is still lacking. This is more a suggestion for future scientific work, as currently we still see studies of jet break-up or dispersion at room temperature. But then spray models are applied at high ambient temperature. Thus, considering the mechanical actions occurring in the vicinity of the nozzle decoupled from the thermal effects which are assumed to be delayed. This has not been proved well. Also, current phase change models in Eulerian framework, like the HRM, are not adequate for evaporation and can’t be used for that purpose.
* Hopefully, experimental measurements (optical, x-ray, …) on OME-3 will be conducted in the future. The intact core length and droplet sizes are currently not known with OME-3.
* High chamber pressure also demands for more systematic investigations on real-fluid effects.
* New fuels to investigate could also include DME, H2 and NH3 (also for compression ignition). Participants seem to demand for that, rather than for nozzle design explorations.
* From the beekast suggestions: aero-related nozzles could also be of great interest for the community, and of great impact, especially if an atomizer is defined.

**Topic 2: Vaporizing spray**

Noud Maes, Eindhoven University of Technology.

Within the vaporizing spray topic, the **main objective was to study mixing differences when moving towards large orifice sprays** (from Spray A with a 90-micron orifice to Spray D with a 190-micron orifice). Additionally, the effect of renewable fuels such as oxymethylene dimethyl ethers (OME) was one of the main interests.

Within this topic there were experimental contributions from 4 institutes, and numerical contributions from 5 institutes. In all cases, experimental data was obtained with dodecane, and OME3-5. For the numerical contributions, benchmark cases with n-dodecane (nC12) were used in most cases. Half of the numerical contributions contained OME3 as a renewable fuel, while the other half performed simulations with OME3-5, either lumping larger OME molecules with OME4, or simulating all of them.

The key take-away messages from this topic were as follows:

* As is evident from the fuel properties, OME fuels will require close to a factor of three less in terms of air entrainment to reach stoichiometry.
* From experimental results published prior to ECN8, it is evident that both the spray penetration and flame lift-off length are similar between nC12 and OME3-5.
* With similar penetration and lift-off length and a much lower stoichiometric air-fuel ratio, much less soot is expected.
* However, at 900 K with Spray D, still some soot is in fact expected (even when using the “atomic oxygen ratio at the lift-off” definition proposed by Mueller et al.).
* A reason why the current guidelines fail to predict the soot tipping-point accurately may be the fact that OME’s do not contain C-C bonds, which is not considered.
* Previous comparisons showed coherence between Rayleigh- and Schlieren-derived penetration, but there were some small discrepancies in the data now that need further checking. Possible explanations could be the 2D vs line-of-sight approach.
* Spray A penetration predictions are much better than those of Spray D: experience?
* However, predictions of the mixture fraction seem very good in both cases.
* While the liquid length of OME3-5 is longer than that of nC12, OME3 seems to show a shorter liquid length.
* Because of a higher mass flow rate in case of OME fuels, the mixture fraction values are consistently higher when compared to nC12.
* When comparing the scalar dissipation rates based on the mixture fraction results, Spray A & D seem to behave similarly regardless of the fuel.
* The scalar dissipation rate predicted from numerical simulations seems to indicate thinner structures than those observed in experiments. There is some discussion on resolution, and down sampling the data in future work to quantify the effect of resolution.

**Topic 3: Ignition**

José M García-Oliver, CMT-UPV.

The aim of this topic was to ***evaluate the ignition sequence and timing (Ignition Delay ID) of the large-orifice Spray D (SD) nozzle under ECN conditions by comparing to Spray A (SA) one***. Especial attention was paid to the fuel effect, particularly to the comparison between dodecane and OME-type fuels. Within this context, published guidelines made up a call for contributions on experiments and simulations with both dodecane and OME3.

Experimental contributions from 3 institutions and numerical results from 6 institutions (most of them with LES approach) were received. No institution performed measurements with OME3 fuel, while a multicomponent OME fuel was available at all institutions from the same supplier and was eventually used in the experiments. This made experimental and numerical comparisons with that fuel possible. In summary, ***most of the analysis was performed based upon a combination of two fuels (C12/OME) and two nozzles (SA/SD) for the nominal conditions****.* Temperature sweeps were used only for experiments, while CFD results were only compared at nominal temperature.

KEY MESSAGES:

* Although not many new experiments were produced, an overall consistency was observed among institutions for ID, except at low temperature, where discrepancies are observed to be more important for dodecane. Such differences were not observed for OME. Consistently with previous results, ignition delay with SD was longer than with SA.
* As for dodecane, good CFD predictions were achieved for SA in terms of ignition delay. This could be expected based upon the previous experience in ECN on the smaller nozzle. A lower degree of accuracy was observed for SD. None of the modelling approaches fully captured the shift from SA to SD, with CFD showing relatively smaller differences than experiments between both nozzles.
* CFD results showed that local ignition in terms of maximum temperature occurs at similar mixture fraction values, irrespective of SA or SD. OME evolutions showed a single-step ignition process, which was justified by canonical flamelet calculations.
* On the other hand, CH2O evolution as derived from high-speed LIF or CFD also hinted at the same ignition events for both SA and SD but with different timings. LES Well-mixed vs UFPV show similar CH2O distribution but different maximum values.
* Flamelet analysis evidenced differences between the two existing OME mechanisms (Cai et al 2020, Niu et al 2021). CFD simulations also confirmed the earlier reaction with Niu.

CONCLUSIONS:

* Both experiments and simulations show ignition of SD further upstream of the jet tip, even from the start low temperature stages
* Modelling captures some of the trends during ignition, but nozzle and fuel effect still need some work to improve ignition predictions.
* Special attention is needed with OME fuels regarding the chemical mechanism due to the discrepancies observed with the available ones. Even though OME was a multicomponent fuel blending OME3-4-5-6, simulations with only OME3-4 seemed to deliver good prediction capability.
* More experiments are needed. High speed CH2O has proved to be a really interesting tool for ignition analysis. New diagnostics, such as high-speed Rayleigh molecular breakdown can also be of interest.

**Topic 4: Flame morphology and emissions**

Julien Manin, Sandia National Laboratories

The objective of this topic was to investigate the flame morphology and emissions for high-pressure spray flames in the context of compression-ignition combustion systems. The guidelines called for large nozzles (Spray D and multi-hole-chicken-foot injectors), moving away from Spray A because of the drastic shift in funding for light-duty applications. While the multi-hole injector was part of the guidelines, no institution performed measurements or simulations, so most of the data were for Spray D. A big emphasis on alternative/sustainable fuels was set as guidelines, with the focus on OME3. N-dodecane (n-C12) fuel was still used in the form of a comparison point.

Technically speaking, the session followed Topic 3 about ignition, with the aim to present information related to lift-off length, flame length and flame structure (OH\*, OH LIF, schlieren, Rayleigh scattering, etc.), as well as emissions with quantitative data about PAHs (LIF, gas-phase sampling), soot (DBI, LII, pyrometry, etc.) and nitrous oxides (LIF, gas-phase sampling).

There were three experimental and four numerical contributions. The experimental work mostly used OME3-5 fuel as opposed to the OME3 requested by the guidelines, and Spray A-3 data were also used as comparisons when experimental measurements for Spray D were lacking.

Below is a summary of key take-away messages from the session:

* More experiments are needed to be conclusive about the flame structure (lift-off length) differences between OME and n-C12 due to the lack of agreement among experimental datasets
* Though overall better than what was observed at ECN 7, the lift-off length for Spray D is still underpredicted by the simulations
* The simulations indicate differences that the detailed mechanisms provided results in better agreement with the experiments
* The well-mixed models provided better agreement with the experiments, even though they do not appropriately capture the flame physics (depending on the resolution)
* Both the experiments and simulations reinforce the strong relationship between low and high temperature reactions
* Looking deeper into the simulation results reveals that CH2O forms in leaner mixtures compared to n-C12, supporting a longer lift-off length for OME
* No soot was detect/measured with OME fuel, even at elevated temperatures like 1200 K
* Unlike the experiments, the simulations show low levels of PAHs and soot with OME

A few general comments and conclusions about the session:

* The session successfully presented comparisons between n-C12 and OME for large nozzles
* Alternative/sustainable fuels can offer soot-free combustion at virtually all relevant conditions
* Understanding low-temperature reactions is key to flame morphology and heat release
* Unfortunately, the session was weak on soot simulation results, and other emissions were neither measured nor simulated by the contributors

The results of the survey highlighted the new reality for engine research:

* Interest in compression-ignition research is strongly associated with sustainable fuels
* Fundamental research appears to attract more participants’ interest (Spray D vs. multi-hole)
* The shift to sustainable fuels (OME, H2, NH3, etc.) brings new challenges (potentially soot free, but hard to ignite or burn) to heavy-duty and off-road applications