

## ECN Modeling Web-meeting

- November 15<sup>th</sup> 2011

**List of participants:** Lyle Pickett (Sandia), Yue Wang (UW-ERC), Adam Dempsey (UW-ERC), Xue-Song Bai (Lund), Zhi Wang, Bruno Kerschgens (RWTH Aachen), David P. Schmidt (UMASS), Sukanta Rakshit (UMASS), Chris Rutland (UW-ERC), Gianluca DErrico (Polimi), Manolis Gavaises (City University), John Abraham (Purdue), Mani Sarathy (Lawrence Livermore NL), Xiaogang Zhang (FORD), Ronald Grover (GM), Jose M. Pastor (CMT), Dan Haworth (Penn State), Bart Somers (TU Eindhoven), Luca Marchitto (Istituto Motori CNR), Sibendu Som (Argonne NL), Nam Cho (John Deere), Yuanjiang Pei (UNSW), Haiwen Ge (FORD), Michele Bolla (ETH-Zurich), Yuri M. Wright (ETH-Zurich), Julien Manin (Sandia), Evatt Hawkes (UNSW), Ossi Kaario (Aalto University)

### Meeting Agenda:

- 1) Introductions by all attendees
- 2) Lyle Pickett: Overview of ECN
- 3) Outcomes of ECN1
  - Sibendu Som to discuss Spray A
  - Evatt Hawkes to discuss n-heptane
- 4) Updates
  - All participants have a chance to present a short update if they wish
- 5) Progress in implementing standard definitions
  - Anybody who has looked at this can contribute
- 6) Chemistry for spray A
  - Sibendu to present the dodecane mechanism
  - A few groups have indicated they have some chemistry developments - need to ask around
- 7) Opportunities for sharing
- 8) Next steps and ECN2.

## Meeting Minutes

*Agenda item 1:* All the participants first introduced themselves and their interest in ECN.

The following questions and answers were discussed during *Agenda items 2 and 3*.

- 1) Sukanta Rakshit: Is the information for internal nozzle geometry measurements, needle-lift available for nozzle flow modeling?

Lyle Pickett: The needle-lift information is available from Argonne National Laboratory. The nozzle internal geometry (actual and nominal) is available from tomography measurements in Caterpillar and CMT-Valencia. Rate of injection results are available from CMT-Valencia. All this information is available from the website from proceedings of ECN1.

- 2) Mani Sarathy: What are the plans for combustion modeling with Spray A?

Sibendu Som: In ECN1, due to the lack of a reliable n-dodecane reduced chemical kinetic model, the focus was to perform non-combustion simulations only. With the new 103-species n-dodecane mechanism developed at Argonne NL in collaboration with Lawrence Livermore NL and University of Connecticut, it may be possible to perform combustion simulations also in the future.

- 3) X.-S. Bai: Is the Lu et al. mechanism for n-heptane relevant for Diesel or HCCI conditions?

Evatt Hawkes: **Action item** to contact Prof. T.F. Lu at University of Connecticut to check if the mechanism was for diesel or fuel lean conditions.

**Follow ups:**

- From Lu *et al.* Combustion and Flame 156 (2009) 1542–1551, “Briefly, the reduction was performed over the parameter range of equivalence ratio 0.5–1.5, pressure 10–50 atm, and initial temperature 700–1600 K for ignition.”
- UNSW results with a well-mixed model and this mechanism were improved over previous results with a much smaller mechanism meant only for high temperature conditions (Patel et al. “ERC” 29-species mechanism).

- 4) Haiwen Ge: Please describe the “well-mixed” model

Evatt Hawkes: Explained the basic functioning of a well-mixed model.

- 5) Mani Sarathy: How as lift-off length determined from OH contours in simulations?

Evatt Hawkes: The LOL was determined based on different definitions by different groups. However, new standardized definitions have now been proposed and are now available in the website.

- 6) Bart Somers: Instead of OH profiles, OH\* profiles need to be looked at. Any mechanisms for OH\* formation available?

Sibendu Som: Showed OH\* results for biodiesel fuel. These simulations were done on a biodiesel skeletal mechanism. Results show significant differences on OH\* and OH mass fraction levels. OH\* mass fractions are in the order of E-10 whereas OH are E-3. Action item: **Action item:** Sibendu will send the OH\* formation reactions that he has implemented in the past.

Mani Sarathy: Need to be careful in drawing any major conclusions from these results since the skeletal model although has OH and CH, make have eliminated important reactions pathways for these species during the reduction process.

*Agenda item 4:* Updates were provided by David Schmidt, Bart Somers, Evatt Hawkes, Dan Haworth

- a) David Schmidt's presentation: While n-heptane was observed to cavitates, dodecane does not cavitate much at all. However, in the real case, n-dodecane could still cavitate due to surface roughness of the nozzle. Simulations were performed with the actual geometry from the mould. David also agreed to provide the geometry to interested modelers.

- 1) Do you simulate the transience of the needle lift simulations?
- 2) Why is the density at the nozzle exit so high and comparable to fuel density?
- 3) Have you compared these simulation results to experimental data?

Manolis Gavaises: Is there value in making a transparent scaled-up nozzle geometry and perform experiments/imaging of cavitation?

Lyle Pickett: Yes, that will be a great value addition. **Action item:** Lyle to contact Manolis to discuss this issue further.

**Action item:** Manolis will contact David to get gambit mesh.

- b) Bart Somers presentation: Progress with LES work using 21% O<sub>2</sub> with n-heptane was shown

c) Evatt Hawkes presentation:

Progress on turbulence-chemistry interactions.

-Using Fluent's transported PDF method. Good agreement for spatial and temporal variations of mean mixture fraction. Not sensitive to mixing model. Mixture-fraction variance is more sensitive. Good agreement can be obtained for  $X > 25\text{mm}$ . Discrepancy of model and experiment near the nozzle  $X < 25\text{mm}$ . Experiment shows non-monotonic trend which is not expected after the liquid length. Lyle Pickett commented that this could be statistical uncertainty. Later follow up modelling the mixture-fraction PDF as Gaussian and using a chi-squared estimate of the 95% confidence interval of the variance has indicated the discrepancy is larger than statistical uncertainty. A systematic measurement error or failing of the modelling is indicated.

-Reacting cases are in progress. Results are very different between the well-mixed model and the PDF model. Results are not yet actually better with the PDF model.

d) Dan Haworth presentation: Mainly comparing well-mixed models with TCI models using PDF methods (Lagrangian particle method versus stochastic fields method) using OpenFOAM and STAR-CD and 2 equation soot model

*Agenda item 5: Evatt Hawkes, Gianluca D'Errico*

a) Evatt Hawkes presentation:

Progress on implementing the ECN1 definitions:

- Vapor-penetration of 0.1% fuel mass fraction appears to work well. Not very sensitive to mesh.
- Liquid penetration definition of 0.15% volume fraction was also mesh independent and agrees with other definitions, surprisingly. This needs to be tested in other solvers (see b)).
- Lift-off length definition of mean  $Y_{OH} = 0.00025$  is not good. Sometimes  $Y_{OH}$  never exceeds this threshold. Particularly for models which are not well-mixed.

Lyle Pickett: Should not choose only one value of OH for representing LOL since the OH concentration changes a lot with O<sub>2</sub> concentration or ambient temperatures.

UNSW Follow up: 2% of the maximum value over the whole domain is a better definition and is more consistent with the experimental definition. LOL is then always defined unless there is no ignition in the simulation.

b) Gianluca D'Errico:

- 1) Definitions are very much dependent on the mesh which is in direct contradiction to Evatt's observations. This needs more discussion and thoughts.
- 2) LOL definition results are with well-mixed models. Iso-temperature of 1600K and IsoOH 0.00025 are seen to be very close to each other.

Lyle Pickett: Need to carry along a length scale along with the liquid volume fraction criterion. Extinction is along a certain length scale.

*Summary and recommendations agenda item 5:*

- 0.1% mixture fraction is good for vapor penetration.
- 0.00025 OH mass fraction is not good for lift-off length. 2% of the maximum in the domain is proposed.
- 0.15% liquid volume fraction for liquid length is controversial. Needs further discussion.
- ignition delay was not discussed.

*Agenda item 6:*

Sibendu Som presented results with the dodecane chemical kinetic mechanism

- 1) 103-species dodecane mechanism was developed from the LLNL mechanism with 2115 species.
- 2) The mechanism seemed to perform well at high temperatures but at low temperature like 800K it tends to overpredict ignition delay. At 750K it did not even predict ignition
- 3) Jetsurf mechanism was also tried but low-T ignition was not well captured
- 4) Further reduction to 50-60 species may be attempted in future

Lyle Pickett: How was the LOL defined? Try doing a line-of-sight approach and vary definitions based on ambient temperatures. Such an approach may better predict LOL.

Gianluca D'Errico, Bart Somers are interested in using the mechanism.

**Action item:** Sibendu will send the 103-species mechanism to Gianluca and Bart.

*Final comments:*

- 1) Update pdf of all presentations made to the ECN website. **Action item:** Lyle will send the username and password for this website.
- 2) **Action item:** Evatt and Sibendu will circulate meeting minutes.
- 3) **Action item:** Can any CFD modeler take ownership of the "modeling standards" section?
- 4) Recording link of the 2.5 hours meeting is given below:  
<https://odt.webex.com/odt/ldr.php?AT=pb&SP=MC&rID=59237252&rKey=2c5ecf60591e17a7>