Topic 1: Internal Flow, Near-Nozzle Break-up, Mixing, and Evaporation

Guidance on Experiments and Simulations to be Performed

Sibendu Som: Argonne National Laboratory

January 24th 2014
Topics of Interest

Topic 1.1: In-nozzle experiments and simulations
Topic 1.2: Near field spray development and coupled nozzle flow and spray simulations
Topic 1.3: Evaporation and Parametric Variations

Bridging the gap: How spray details (Topic 1) affect Combustion (Topic 2)
Topic 1.1: In-nozzle Experiments and Simulations

David Schmidt: University of Massachusetts
Chris Powell*: Argonne National Laboratory
Experimental Objectives

• Provide boundary conditions for simulations of internal flow
  – Nozzle geometry
  – Rate of injection
  – Needle lift & off-axis motion

• Provide data for validation
  – Radiography at nozzle exit
  – Nozzle flow coefficients

• Assess the uncertainties for all of these parameters
Modeling Objectives

• Define level of confidence of internal flow simulations by validating, where possible, with experimental data
• Quantify internal flow dynamics that are likely to affect spray characteristics of primary atomization
• Assess which physical phenomena are important for including in models
  – Turbulence
  – Compressibility
  – Equilibrium vs. non-equilibrium phase change
  – Dissolved or non-condensable gasses
• Quantities to be compared for validation:
  – Cd, Cv, Ca (for each hole, in the case of spray-B).
Target Injectors

• Spray A
  – Diesel nozzle, single hole, n-dodecane, non-cavitating
  – High resolution (1 mm) X-ray tomography of Nozzle 675
  – Ultra High resolution (0.6 mm) tomography for 678, & 679
  – Lift and wobble measured for all nozzles
  – The target injector will be 675

• Spray B
  – Diesel nozzle, 3-hole, n-dodecane, non-cavitating
  – Ultra High resolution (0.6 μm) tomography partially completed
  – Lift and wobble measured for 199, 200 but not yet 201 (use 199 lift and wobble profile for simulations)
  – The target injector will be 201
Priority List: Simulations

• Spray A conditions:
  – Injector 675
  – 150 MPa injection pressure vs. time (BoundaryCondition&Data.zip)
  – 100 MPa injection pressure vs. time (BoundaryCondition&Data.zip)
  – Fuel temperature 343 K

• Spray B conditions:
  – Injector 201
  – 150 MPa injection pressure (injection pressure vs. time: Use same as Spray A)
  – 100 MPa (second priority: Use same as Spray A)
  – Fuel temperature 338 K
Data Needed from Experiments

• Dissolved gas content (assume the equilibrium value of 1.28E-3 mole fraction)

• Mass flow rate at the nozzle exit*
  • Spray A target injector
    • Long tube method for ROI
    • Momentum measurements
    • Virtual Injection Rate Generator: http://www.cmt.upv.es/ECN03.aspx
      • Preferred for simulations, data already available
  • Spray B target injector
    • ROI for each hole, individually
    • Virtual Injection Rate Generator: http://www.cmt.upv.es/ECN03.aspx
      • Preferred for simulations, data available end of January

• Needle motion and wobble*
  – Spray A (BoundaryCondition&Data.zip)
  – Spray B (BoundaryCondition&Data.zip)

* These data are provided prior to the simulations being run
Data Needed from Simulations

• Spray A target injector
  – Mass and momentum flow rate and fluctuation distribution at the nozzle exit vs. time
  – Axial slices showing transverse variation of mass flow and momentum at exit for $\theta = 0^\circ$. Radial distribution of mass flow and momentum along this axial slice
  – $C_d$, $C_v$, $C_a$

• Spray B target injector
  • Mass and momentum flow rate and fluctuation distribution at the nozzle exit vs. time
  • Axial slices showing transverse variation of mass flow and momentum at exit for $\theta = 0^\circ$. Radial distribution of mass flow and momentum along this axial slice
  • $C_d$, $C_v$, $C_a$ for each hole
  • Flow split between holes vs. time
  • Vapor fraction at the exit plane as a function of time
  • Iso-surface of 50% vapor by volume
Deadlines

• Experimental data
  – Need ROI (slide 8), geometry (slide 6), and needle motion (slide 8) by January 25
  – Data for validation by March 1
  – Guidelines on how to submit results will be provided shortly
  – Data should be submitted to Chris Powell (cpowell@anl.gov) and cc to Sibendu Som (ssom@anl.gov)

• Computational results:
  – All results must be provided by March 1
  – Guidelines on how to submit results will be provided shortly
  – Data should be submitted to David P. Schmidt (schmidt@ecs.umass.edu) and cc to Sibendu Som (ssom@anl.gov)
Topic 1.2: Near field spray development and coupled nozzle flow and spray simulations

Alan Kastengren*: Argonne National Laboratory
Qingluan Xue: Argonne National Laboratory
Julien Manin: Sandia National Laboratory
Chawki Habchi: IFPEN
Objectives

• Focus on the near nozzle region within first 10 mm
• Obtain quantitative (fuel concentration, droplet size, etc.) and qualitative (macroscopic parameters, optical/x-ray relationship, etc.) information about the breakup process of sprays
• Provide high-fidelity measurements of liquid penetration, liquid mass distribution, and droplet size in the nozzle near field
• Facilitate dynamic coupling of in-nozzle flow and external spray approaches
• Compare the different coupling approaches of in-nozzle flow and external spray
• Encourage high-fidelity simulations near nozzle sprays and liquid jet atomization
• Study the capability of the different modeling approaches (Lagrangian-Eulerian, Eulerian-Eulerian) and CFD frameworks (RANS, LES, DNS) for the simulation of the primary atomization and the cavitation
Anticipated Experimental Results

- Imaging of internal nozzle gas flow and near-nozzle dribble with x-ray phase-contrast imaging
- Microscopic measurements of the initial penetration and spreading angle
- Break up and mixing of the sprays at the end of injection at the microscopic level
- USAXS droplet sizing and perhaps optically measured droplet size as well
- X-ray radiography of Spray B: nozzles 199 and 201
- Ballistic imaging of near-nozzle region
Priority List – Spray A Simulations

• Spray of interest: injector 675
• Condition # 1: Non-evaporating conditions from x-ray radiography at Argonne
  • Ambient pressure: 2 MPa; Ambient temperature with pure N\textsubscript{2}: 303 K
  • Injection pressure: 150 MPa; Fuel injection tip temperature: 343 K
• Condition # 2: Parametric variation on Condition #1
  • Ambient pressure: 2 MPa; Ambient temperature with pure N\textsubscript{2}: 303 K
  • Injection pressure: 100 MPa; Fuel injection tip temperature: 343 K
• Spray of interest: Injector 201, plume #3
• Condition # 1, non-evaporating conditions from x-ray measurement at ANL
  • Ambient pressure: 2.01 MPa; Ambient temperature with pure N2: 306 K
  • Injection pressure: 155 MPa; Fuel injection tip temperature: 338 K
• Condition # 2, non-evaporating conditions from x-ray measurement at ANL
  • Ambient pressure: 2 MPa; Ambient temperature with N2: 306 K
  • Injection pressure: 100 MPa; Fuel injection temperature: 338 K
Data Needed from Experiments

- Data needed for initializing Spray A and Spray B simulations are already highlighted in Topic 1.1
- For both injectors: (Data available: BoundaryCondition&Data.zip)
  - Mass flow rate at the nozzle exit from virtual ROI tool from CMT and measured nozzle coefficients
  - Fuel spray penetration vs. time from long-distance microscopy and diffused back-illumination
  - Contour plots of projected liquid density at 0.1 ms and 0.5 ms from Argonne
  - Transverse mass distribution (projected density across the spray) profiles averaged between 0.5 – 1.0 ms:
    - $x = 0.1, 0.6, 2, 6, \text{ and } 10 \text{ mm downstream to nozzle exit}$
    - Projection plane is 0° plane (i.e., plane containing fuel inlet, or projection along the z-axis with the injector in the theta = 0 position)
  - Transverse integrated mass (TIM) vs. axial distance in the near nozzle region @ 0.5 ms
- For Spray A:
  - Liquid volume fraction across cross-section at $x = 0.1, 0.6, 2, 6, 10 \text{ mm}$
  - the y-axis cut plane (check slide 17)
Near-nozzle comparisons

- Much different results if comparing mixture fraction or liquid volume fraction.
- LVF or mixture fraction data derived from x-ray measurements (see SAE 2014-01-1412) compared to a model:

![Diagram showing liquid volume fraction (LVF) profiles and model mixture fraction comparison.](image-url)
Data Needed from Spray A Simulations

- Mass flow rate at the nozzle exit
- Fuel spray penetration vs. time (0.1% liquid mass fraction)
- Contour plots of projected density in the 0° plane at 0.1 and 0.5 ms after actual SOI
- Projected fuel mass/density (ug/mm²) profiles across nozzle axis at 0.5 ms after SOI
  - x = 0.1, 0.6, 2, 6, and 10 mm downstream to nozzle exit
  - @ x= 0.6 and 6 mm, @ 0.75 ms and 1 ms after SOI
- 2D contours of liquid volume fraction at x = 0.1, 0.6, 2, 6, 10 mm
- Transverse integrated mass profiles at 0.5 ms after SOI:
  - x = 0.1 mm, 0.6 mm, 2 mm, 6 mm, and 10 mm
- Mean droplet size (SMD) at x = 1, 4, 8 mm at 0.5 ms after SOI
  - Mean SMD at the above axial positions vs. axial position
  - Distributions of SMD vs. radial position at the above axial positions
- Dynamics: peak projected density and Full Width Half Maximum (FWHM) of distribution at x = 0.1, 2, 6 mm from nozzle for entire duration of the injection event (in intervals of 20 μs)
Data Needed from Spray B Simulations

- **Spray B target injector (201):**
  - Compare results between different plumes for condition #1
    - Penetration vs. time
    - Transverse mass distribution at 0.1 mm, 2 mm, and 6 mm
    - Mean SMD at 1, 4 mm at 0.5 ms after SOI vs. axial position

- **For plume #3 which is measured at Argonne**
  - Contour plots of projected density in the 0° plane at 0.1 and 0.5 ms after actual SOI
  - Projected fuel mass/density (ug/mm²) profiles across nozzle axis at 0.5 ms after SOI
    - x = 0.1, 0.6, 2, 6, and 10 mm downstream to nozzle exit
    - @ x = 0.6 and 6 mm, @ 0.75 ms and 1 ms after SOI
  - 2D contours of liquid volume fraction at x = 0.1, 0.6, 2, 6, 10 mm
  - Transverse integrated mass profiles at 0.5 ms after SOI:
    - x = 0.1 mm, 0.6 mm, 2 mm, 6 mm, and 10 mm
  - Mean droplet size (SMD) at x = 1, 4, 8 mm at 0.5 ms after SOI
    - Mean SMD at the above axial positions vs. axial position
    - Distributions of SMD vs. radial position at the above axial positions
Deadlines

• Computational results:
  – January 25, 2014: model input data provided
  – February 15, 2014: contact organizers to arrange data format for submission
  – March 1, 2014: all results must be submitted
  – Results should be submitted to:
    – Alan Kastengren (akastengren@anl.gov)
    – Julien Manin (jmanin@sandia.gov)
    – Qingluan Xue (qxue@anl.gov)
    – Chawki Habchi (chawki.habchi@ifpen.fr)
    – Sibendu Som (ssom@anl.gov)
Topic 1.3: Evaporation and Parametric Variations

Alessandro Montanaro: – CNR Instituto Motori
Tommaso Lucchini*: – Politecnico di Milano
Global Objectives

• Focus on non-combusting conditions

• Understanding how the spray development in the far field is influenced by variation of operating conditions:
  • Injection pressure
  • Ambient density
  • Ambient temperature
  • Nozzle geometry

• How different experimental techniques affect measurements?

• Are multi-dimensional models capable to reproduce experimental trends?
Objectives

**Experimental:**
- Define a set of operating conditions to build a database of experiments for Spray-B configuration.
- Understanding how results are repeatable in different institutions (Spray A and Spray B).
- Understanding influence of different nozzle serial numbers on spray evolution (Spray A and Spray B).

**Simulation:**
- How different models reproduce the effects of different operating conditions on spray evolution?
- To compare different approaches (Eulerian-Lagrangian, Eulerian-Eulerian, ...) and, within the same approach, different sub-models.
- Understanding how spray evolution from multi-hole nozzle is affected by mesh structure.
<table>
<thead>
<tr>
<th>Priority level</th>
<th>T [K]</th>
<th>density [kg/m$^3$]</th>
<th>Pressure [MPa]</th>
<th>Fuel</th>
<th>T fuel [K]</th>
<th>Injection duration [ms]</th>
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</table>
Required Experimental data for Spray-A

Experimental data to be provided

- Injected fuel mass flow rate
- Liquid spray penetration versus time
- Liquid spray penetration (steady)
- Vapor penetration versus time
- Radial distribution of mixture fraction and variance at 25 and 45 mm from injector at 1.5 ms after SOI.
- Axial distribution of mixture fraction and variance at 1.5 ms after SOI.
- Radial distribution of axial and radial velocity components at 25 and 45 mm from injector at 1.5 ms after SOI.
- Axial velocity distribution at 1.5 ms after SOI.

Additional information (only if it is different from Spray A)

- Details about the used test-rig.
- Details about vessel temperature distribution at start of injection.
- Details about techniques used for experiments.
• Ambient conditions: use SANDIA ECN experimental data search utility.
• Injected mass flow rate profile: use CMT mass flow rate generator.
• Nozzle geometry: use 675 dimensions
• Tune the model on baseline Spray A condition (priority 1) with 1.5 ms injection duration.
Required Data from Spray A simulations

Simulated operating points: same of experiments

Simulated data to be provided

- Liquid spray penetration versus time
- Liquid spray penetration (steady)
- Vapor penetration versus time
- Radial distribution of mixture fraction and variance at 0.1, 0.6, 2, 5, 6, 10, 25, and 45 mm from injector at 1.5 ms after SOI
  - Vapor-phase and total (liquid and vapor) mixture fraction.
  - For only priority 1, 6, 10 (in slide 24)
- Axial distribution of mixture fraction and variance along the centerline at 1.5 ms after SOI.
- Radial distribution of axial and radial velocity components at 0.6, 5, 10, 25 and 45 mm from injector at 1.5 ms after SOI
  - For only priority 1, 6, 10 (in slide 24)
- Axial velocity distribution at 1.5 ms after SOI.
### Experimental Data Requested for Spray-B*

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<th>density [kg/m³]</th>
<th>Pressure [MPa]</th>
<th>Fuel</th>
<th>T fuel [K]</th>
<th>Injection duration [ms]</th>
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* It is understood that all the above Spray B data may not be available by March 1st, hence please plan your experiments as per the noted priority.

### Experimental data to be provided
- Injected fuel mass flow rate: available from the virtual rate generator at CMT
- Liquid spray penetration versus time
- Liquid spray penetration (steady)
- Vapor penetration versus time

### Additional information
- Details about the used test-rig
- Details about vessel temperature distribution at start of injection
- Details about techniques used for experiments
• Ambient conditions: use SANDIA ECN experimental data search utility.
• Injected mass flow rate profile: use CMT rate of injection generator
• Nozzle geometry specifications for 201
• Use the same set of model constant that were obtained for Spray A baseline condition
Spray B simulations

Objective: understanding how mesh structure affects spray evolution.

- All three holes must be included in simulations
- Use same spray parameters from spray A model tuning

Simulated operating points

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<th>Priority level</th>
<th>T [K]</th>
<th>density [kg/m³]</th>
<th>Pressure [MPa]</th>
<th>Fuel</th>
<th>T fuel [K]</th>
<th>Injection duration [ms]</th>
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<td>150</td>
<td>n-dodecane</td>
<td>363</td>
<td>1.5</td>
</tr>
</tbody>
</table>
Required Data from Spray B simulations

- Liquid spray penetration versus time for each plume
- Liquid spray penetration (steady) for each plume
- Vapor penetration for each plume
- Projected gas velocity along the axis of each plume
- Radial velocity distribution for each plume at 2, 10, and 20 mm axial distance from nozzle.
- Radial mixture fraction distribution for each plume at 2, 10, and 20 mm axial distance from nozzle.
- Radial mixture fraction variance distribution for each plume at 2, 10, and 20 mm axial distance from nozzle.
Deadlines

• Computational and experimental results:
  – Contact organizers by **February 15th** for data submission format
  – All results must be provided by **March 1st**
  – Experimental results to be sent to Alessandro Montanaro (alemon@im.cnr.it) and cc to Sibendu Som (ssom@anl.gov)
  – Simulation results should be sent to Tommaso Lucchini and Roberto Torelli (tommaso.lucchini@polimi.it, roberto.torelli@polimi.it) and cc to Sibendu Som (ssom@anl.gov)
Bridging the gap: How Spray details (Topic 1) affect Combustion (Topic 2)

Yuanjiang Pei, Sibendu Som: Argonne National Laboratory
Jose Garcia: CMT-Motores Termicos
Objectives

- Designed to bridge-the-gap between spray (Topic 1) and combustion (Topic 2) for Spray A
- How do the differences in boundary conditions and spray characteristics influence combustion characteristics?
- Can simulations using the best boundary conditions available, capture these trends?
- Why differences in spray characteristics do not seem to influence the combustion behavior?
- What are the most sensitive variables for different targets of spray and combustion characteristics? - (Global Sensitivity Analysis)
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<td>O₂=0; N₂=89.71; CO₂=6.52; H₂O=3.77</td>
<td>O₂=15; N₂=75.15; CO₂=6.22; H₂O=3.62</td>
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- For injection parameters, one can choose injection pressure or mass injected and injection duration, you may choose the one that suits your need.
- OH mole fraction is obtained from Nesbitt et al. 2011, approximations are made.
- Run 3 simulations with nominal, SNL and CMT on each conditions listed below, and use the available boundary conditions (cf. Slide 3) to capture the variation of the experiments.
  - One non-reacting case at 900 K
  - Three ambient T conditions for reacting cases, 800 K, 900 K and 1100 K.
- **Submit the following results using recommended definitions by each topic organizer:**
  - Global Sauter mean diameter vs. time
  - Liquid length vs. time
  - Vapor penetration length vs. time
  - Lift-off length vs. time
  - Ignition delay
  - Modeling and numerical details provided to each topic organizer i.e., Sibendu Som and Jose Garcia
  - Please report the boundary conditions you used that are different than the ones listed in the table of last slide in any case.
- **Additional data may be requested based on analysis to gain further insight**
• Submission deadline: March 1st 2014
• Please send the data to Yuanjiang Pei (ypei@anl.gov)
• Format for the data submission (both line and contour plots) will be made available soon