TOPIC 2
PRIMARY ATOMIZATION (NEAR-NOZZLE MIXING)

Presenter: Michele Battistoni, University of Perugia
Valencia, September 10th, 2018

Contributors (list of groups):
Experiments:
- Shane Daly, Oregon State, - Scott Skeen, Emre Cenker, Lyle Pickett, Sandia National Laboratories - Cyril Crua, Univ. Brighton - Fredrik Westlye, Tech Univ. Denmark - Julien Manin, Artium
- Brandon Sforzo, Alan Kastengren, Katie Matusik, Chris Powell, Argonne National Laboratory,
Simulations:
- Marco Arienti, Joonsik Hwang, Sandia National Laboratories
- Michele Battistoni, University of Perugia
- Mathis Bode, Aachen University
- José M. Pastor, CMT - Adrian Pandal, University of Oviedo, - Bertrand Naud, Ciemat
- Aqeel Ahmed, François-Xavier Demoulin, Coria
- Julien Manin, SANDIA, Artium
- Peetak Mitra, David Schmidt, University of Massachusetts
More and more simulations consider both nozzle internal flow and near-field flow and how this affects spray characteristics:
- This allows proper boundary conditions
- Transient effects can be tackled
- Focusing on either nozzle internal flow or near-field flow only seems questionable (possibly, same simulation for two topics)

Three different nozzles available: Spray A, C, D
- With known boundary conditions:
  - real geometries, needle tip motion, wall temperatures
OBJECTIVES

• Focus on the near-nozzle region: **within first ~10 mm**
  • Spray A
  • Spray C / D

• Capture spray physics under nominal ECN conditions and under cold conditions

• Study and comparison of different modeling approaches, from RANS to LES, to DNS, and Lagrangian-Eulerian, Eulerian-Eulerian

• Encourage high-fidelity simulations of fuel sprays to understand the physics of the primary atomization

• Provide a robust database for model validation and for physics understanding
  • mass distribution
  • phase interfacial area
  • droplet sizing
## CONTRIBUTORS – EXPERIMENTS

<table>
<thead>
<tr>
<th>Group</th>
<th>Spray</th>
<th>Data &amp; Conditions</th>
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<tbody>
<tr>
<td><strong>ANL (US)</strong></td>
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<tr>
<td>Brandon Sforzo, Katarzyna Matusik, Christopher Powell, Alan Kastengren</td>
<td>A ✓ ✓ ✓</td>
<td>Radiography - spray A #675 ref. case + parametric variations, - spray C #37 ref. case, - spray D #133 ref. case + parametric variations, - spray D #134 ref. case</td>
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<tr>
<td><strong>SANDIA (US)</strong></td>
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<tr>
<td>Shane Daly, Oregon State Scott Skeen, Emre Cenker, Lyle Pickett, Sandia National Laboratories Cyril Crua, Univ. Brighton Fredrik Westlye, Tech Univ. Denmark Julien Manin, Artium</td>
<td>✓ ✓ ✓</td>
<td>Optical long-distance microscopy</td>
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<td></td>
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<td>Measurement of liquid envelope for Spray C and Spray D with different fuel and ambient temperatures</td>
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## CONTRIBUTORS – CFD MODELERS

<table>
<thead>
<tr>
<th>Institution/Group</th>
<th>Spray</th>
<th>Conditions: Steady state/Transient/…</th>
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<tr>
<td>Aachen RWTH (Germany)</td>
<td>Mathis Bode, Marco Davidovic, Heinz Pitsch</td>
<td>A, C, D</td>
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<tr>
<td>CMT-UniOvi-CIEMAT (Spain)</td>
<td>José M. Pastor, Adrian Pandal Blanco, Bertrand Naud</td>
<td>✓</td>
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<tr>
<td>CORIA (France)</td>
<td>Aqeel Ahmed, François-Xavier Demoulin</td>
<td>✓</td>
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<tr>
<td>Perugia (Italy)</td>
<td>Michele Battistoni</td>
<td>✓, ✓</td>
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<tr>
<td>SANDIA (US)</td>
<td>Marco Arienti, Joonsik Hwang</td>
<td>✓</td>
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<td>SANDIA-Artium (US)</td>
<td>Julien Manin</td>
<td>✓</td>
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<td>UMass (US)</td>
<td>Peetak Mitra, Declan Gwynne, Eli Baldwin, David Schmidt</td>
<td>✓, ✓</td>
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## MODEL DESCRIPTION

<table>
<thead>
<tr>
<th>Institution/Group</th>
<th>approach</th>
<th>CFD code</th>
<th>Compressibility and EOS</th>
<th>Turbulence model</th>
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<tbody>
<tr>
<td>Aachen RWTH, Mathis Bode</td>
<td>In-nozzle: LES/Atomiz.: DNS</td>
<td>CIAO (in-house)</td>
<td>Compressible code with HEM with (SG/PR EOS) Low-Mach</td>
<td>LES - Dynamic Smagorinsky, with Lagrangian averaging backward in time</td>
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<td>Marco Davidovic</td>
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<tr>
<td>CMT-UniOvi-CIEMAT, José M. Pastor</td>
<td>Diffuse interface (mixture) + Σ-Y Eulerian single fluid</td>
<td>OpenFOAM</td>
<td>Barotropic liquid Ideal gas</td>
<td>LES eddy viscosity based SIGMA model (Nicoud et al. POF, 2011)</td>
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<td>Adrian Pandal Blanco</td>
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<td>Bertrand Naud</td>
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<td>CORIA, Aqeel Ahmed</td>
<td>Diffuse interface (mixture) + Σ-Y and ELSA model</td>
<td>OpenFOAM</td>
<td>Incompressible</td>
<td>LES WALE</td>
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<tr>
<td>Perugia, Michele Battistoni</td>
<td>1) Diffuse interface (mixture)</td>
<td>CONVERGE</td>
<td>1) barotropic liquid + ideal gas</td>
<td>LES Dynamic Structure</td>
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<td>2) Sharp interface VOF</td>
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<td>2) incompressible</td>
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<td>SANDIA, Marco Arienti, Hwang</td>
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<td>CONVERGE</td>
<td>barotropic liquid + RK gas</td>
<td>RANS RNG k-ε</td>
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<tr>
<td>SANDIA-Artium, Julien Manin</td>
<td>VOF</td>
<td>Gerris</td>
<td>Incompressible</td>
<td>DNS no model</td>
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<td>UMass, Peetak Mitra, Declan Gwynne, Eli Baldwin, David Schmidt</td>
<td>Diffuse interface (mixture) + Σ-Y Homogeneous Relaxation Model Eulerian single fluid</td>
<td>HRM Foam</td>
<td>Compressible Refprop (NIST database)</td>
<td>RANS k-ω</td>
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## MODEL DESCRIPTION

<table>
<thead>
<tr>
<th>Institution/Group</th>
<th>min-max mesh resolution (within the 0-10 mm range)</th>
<th>Needle motion</th>
<th>Internal nozzle included</th>
<th>Dimensionality and domain extension</th>
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<tbody>
<tr>
<td>Aachen RWTH, Mathis Bode Marco Davidovic Heinz Pitsch</td>
<td>1 μm - 60 μm</td>
<td>Moving needle</td>
<td>1-way coupling interface at nozzle exit</td>
<td>3D</td>
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<tr>
<td>CMT-UniOvi-CIEMAT, José M. Pastor Adrian Pandal Blanco Bertrand Naud</td>
<td>3 μm – 90 μm</td>
<td>Fixed – high lift</td>
<td>Not included (educated ROI + synthetic turbulent fluctuations)</td>
<td>3D (chamber L = 20 mm)</td>
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<tr>
<td>CORIA, Aqeel Ahmed François-Xavier Demoulin</td>
<td>1 μm – 15 μm (axisymmetric) 2 μm – 80 μm (STL)</td>
<td>Fixed – high lift</td>
<td>Yes</td>
<td>3D (chamber L = 10 mm)</td>
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<tr>
<td>Perugia, Michele Battistoni</td>
<td>2.5 μm – 40 μm (with AMR)</td>
<td>Fixed – high lift</td>
<td>Yes</td>
<td>3D (chamber L = 15 mm)</td>
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<tr>
<td>SANDIA, Marco Arienti, Hwang</td>
<td>7.81μm - 250μm (with embedded refinements and AMR)</td>
<td>Fixed – high lift</td>
<td>Yes</td>
<td>3D (chamber L = 24 mm)</td>
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<td>SANDIA-Artium, Julien Manin</td>
<td>0.9 μm (0 to 20 diam.) 1.8 μm (0 to 40 diam.) 3.6 μm (0 to 80 diam.)</td>
<td>Fixed – high lift</td>
<td>No internal flow (fixed velocity profile)</td>
<td>3D (20, 40 and 80 diameters long domains)</td>
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<tr>
<td>UMass, Peetak Mitra, Declan Gwynne, Eli Baldwin, David Schmidt</td>
<td>1.1 μm – 25 μm (Pacman mesh motion Library)</td>
<td>C) Fixed – high lift D) Moving needle</td>
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<td>3D (chamber L= 3 mm)</td>
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## MODEL DESCRIPTION

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<th>Spatial discretization</th>
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<td>Aachen RWTH,</td>
<td>A #675</td>
<td>hex</td>
<td>800 M</td>
<td>Hybrid (2nd/4th CD &amp; WENO 3rd/5th)</td>
<td>2nd order Runge-Kutta</td>
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<td>Mathis Bode</td>
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<td>Marco Davidovic</td>
<td>D #134</td>
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<td>Heinz Pitsch</td>
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<td>hex (structured Cartesian)</td>
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<td>CMT-UniOvi-CIEMAT</td>
<td>A #675</td>
<td>hex</td>
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<td>2nd order Gamma NVD</td>
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<td>José M. Pastor</td>
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<td>Blanco Bertrand</td>
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<td>Naud</td>
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<td>CORIA,</td>
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<td>A #675 – high resolution STL</td>
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<td>François-Xavier</td>
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<td>Demoulin</td>
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<td>C #37 – high resolution STL</td>
<td>hex</td>
<td>50 M</td>
<td>1) 2nd order CD for all (with flux limiter), except for turbulence, 2) VOF-LES 1st order</td>
<td>1st order Euler Dt ~ 1.0 ns</td>
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<td>Michele Battistoni</td>
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<td>Coria</td>
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<td>Marco Arienti</td>
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<td>Marco Arienti,</td>
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<td>Hwang</td>
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<td>SANDIA-Artium,</td>
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<td>hex</td>
<td>max 540 M</td>
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<td>Julien Manin</td>
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<td>(Octree with ARM)</td>
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<td>UMass,</td>
<td>C #37 – Wireframe (axisym.)</td>
<td>Polydehra</td>
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<tr>
<td>Declan Gwynne,</td>
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<tr>
<td>Eli Baldwin, David Schmidt</td>
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</table>
SPRAY A

CMT-Universidad de Oviedo-CIEMAT (OpenFOAM – LES)

SANDIA-Artium (Gerris – DNS)

CORIA (OpenFOAM – LES)
SPRAY C/D

Aachen (CIAO – DNS)

SANDIA (CONVERGE – RANS)

Perugia (CONVERGE – LES)

sharp

diffuse

Umass
(HRMFoam – RANS)
SPRAY A – PROJECTED MASS & TRANSV. INTEGRATED MASS (EXP VS. SIM)

LES calculations:
Single realization + time-averaging
Improvements up to 5-6 mm, with LES:
……lack of resolution in the far field? (under-resolved LES?)
Improvements up to 5-6 mm, with LES:
……lack of resolution in the far field? (under-resolved LES?)
SPRAY A – DROPLET SIZE

drop statistics (from DNS in the very early stage – Gerris code)

SANDIA-Artium

-0.2 0 0.2 0.4 0.6 0.8 1
-0.2 0 0.2 0.4 0.6 0.8 1

SMD from DNS is still over-estimated by a factor of about 4X (resolution used was 1um)

• pdf of diameters are still not available from experiments in the dense core for comparison
SPRAY D – PROJECTED MASS & TRANSV. INTEGRATED MASS (EXP)

D #134 0deg

D #133

D #134 90deg

Axial distance [mm]
SPRAY D – PROJECTED MASS & TRANSV. INTEGRATED MASS (EXP VS. SIM)

Perugia (sharp) – not time averaged

Perugia (diffuse)

D #134 0deg

ANL D #134 - 0deg

ANL D #134 - 90deg

TIM [μg/mm]

axial distance [mm]
Spray D #134 jet deviates substantially from the axis.

Models tend to capture the distribution, if a transverse offset is applied.
SPRAY D – PROJECTED FUEL MASS PROFILES (STEADY)

- Re-centering is needed for better comparison, maybe about the FWHM
- Models tend to capture the distribution and details of asymmetries
SPRAY C – PROJECTED FUEL MASS & TRANSVERSE INTEGRATED MASS (EXP)

C #37 0deg

C #37 90deg

z [mm]

0 5 10 15 20 25 30 35 40 45 50

x [mm]

0 2 4 6 8 10 12 14

y [mm]

0 1 2

[μg/mm²]

0 50 100

TIM [Hg/mm]

0 5 10 15 20 25 30 35 40 45

axial distance [mm]

ANL C #37 - 0deg

ANL C #37 - 90deg
SPRAY C – PROJECTED FUEL MASS & TRANSVERSE INTEGRATED MASS (EXP VS. SIM)

Perugia (sharp) – not time averaged

Perugia (diffuse)

SANDIA

C #37 0deg

Aachen
Perugia (diffuse)
C37 SANDIA
ANL C #37 - 0deg
ANL C #37 - 90deg
SPRAY C – PROJECTED FUEL MASS PROFILES (STEADY)

x = 0.1 m

x = 2 m

x = 4 m

x = 6 m

Aachen 0deg
Perugia (diffuse)
SANDIA 0 deg
ANL C #37 - 0deg

μg/mm²

y [mm]

x = 0.1 m

x = 2 m

x = 4 m

x = 6 m

C #37 0deg

μg/mm²
SPRAY C – PROJECTED FUEL MASS PROFILES (STEADY)

Sforzo et. al. ICLASS 2018
SPRAY D_134 vs. C_37: FUEL DENSITY FIELD at \( x = 0.1 \text{ mm} \)

C_37

D_134

ANL reconstructed fuel density field \((\mu g/mm^3)\)

Time averaged in the steady state part

Sforzo et. al. ICLASS 2018
SPRAY C_37: FUEL DENSITY FIELD at x = 0.1, 2, 5 mm

ANL reconstructed fuel density field ($\mu g/mm^3$)

Time averaged in the steady state part

Sforzo et al. ICLASS 2018
SPRAY C_37: FUEL DENSITY FIELD at \( x = 0.1, 2, 5 \text{ mm} \)

0.1 mm

2 mm

5 mm

ANL  Perugia  SANDIA  UMass
SPRAY C/D – INTERFACIAL AREA

Experiments: USAXS (Ultra Small Angle X-ray Scattering)

- Axial sweep
- Transv. sweep

Bin size in the USAXS experiments: 50 µm × 500 µm

In order to compare “apple-to-apple”: Simulation postprocessing that mimicks USAXS method

Total area of phase interface, \( A \), and the total volume, \( V \) with “USAXS-like” method: \( \frac{V}{V_{\text{box}}} \) & \( \frac{A}{V_{\text{box}}} \)

Line-of-sight box, moving along \( X \) and \( Y \), to collect info on each structure, including core

On each box, collection of:
- liquid volume \( V \)
- interface area \( A \)

\[
SMD = 6 \frac{V/V_{\text{box}}}{A/V_{\text{box}}}
\]

Battistoni, Magnotti, et al., SAE 2018

Matusik et. al. ICLASS 2018
Kastengren et al., IJMF 2017
• The double peak in the projected area distribution is due to the intact core.
• It is therefore possible to identify the liquid core length. In this case about 5-6 mm
SPRAY D – SAUTER MEAN DIAMETER

- Model captures the SMD trend
- Actual droplet size (detached structures) is insensitive to the axial distance
- Room for improvement: more resolution still required to be fully predictive at diesel spray conditions
- USAXS data include the liquid core: USAXS provide an apparent SMD in the centerline

Battistoni, Magnotti, et al., SAE 2018

Matusik et. al. ICLASS 2018
SPRAY C VS. D – SAUTER MEAN DIAMETER

**x = 10 mm**

- C has finer structures in the periphery
- C is much more spread along y-dir

Spray centerline (y=0 mm)

- Due to inclusion of core

Projected liquid mass

Perugia (C #37) (sharp) – not time averaged

Atomized region

Intact core
SPRAY C – PROJECTED AREA, MASS, AND SAUTER MEAN DIAMETER

- Area is underestimated, so SMD overestimated, because of grid resolution limit
- The spreading of spray C is larger in y-dir, in accordance with x-ray experiments

0 deg view
SPRAY C – INTERFACIAL AREA PARAMETRIC VARIATIONS

0 deg
(view 1)

1500 - 20 bar

1500 - 1 bar

500 - 1 bar
SPRAY C, 900 K AMBIENT, 440 K FUEL T

- View 2 much more narrow for Spray C
- Spray D the same
- Due to cavitation that causes a large disturbance that creates growth in the View 1 direction
SPRAY C, 900 K AMBIENT, 363 K FUEL T

Center plume and plot data at 2 and 8 mm

Recommendation for CFD comparison

Best estimate for a liquid length threshold, preserving past assumptions:

$$\tau = 0.37 \quad \text{estimated assuming about 2 \( \mu \text{m} \) droplet}$$

$$\tau \frac{\pi d^3/6}{C_{ext}} = \int_{-\infty}^{\infty} LVF \cdot dy = 0.2 \cdot 10^{-3} \ \frac{\text{mm}^3\text{liquid}}{\text{mm}^2}$$

- Need to test Eulerian models with this criteria
- Assess the assumptions, like 2 \( \mu \text{m} \) at different p,T
SOME FUTURE DIRECTIONS

- Need to validate liquid dispersion and atomization (like Σ-Y, or other models) on C/D, rather than on A. There is more knowledge now and more spatially varying dataset available on C/D.

- Need to check better the phase interaction (drag,...) in Eulerian formulation, with reference to turbulence models, and atomization (bi-directional effects should be included).

- Focus on the core and detached structures, being aware of the value interpretation.

- Test projected liquid volume (PLV) criterion to detect spray boundary (angle or penetration): compare models vs. optical measurements and mass-based measurements.

- Temperature of the fuel, temperature of the chamber

- Since most of the model development (or tuning) is based on mass-based measurements, it would be very important to quantify uncertainties (error bars) or define specific known test cases.