Simulation of Liquid and Gas Phase Characteristics of Aerated-Liquid Jets in Quiescent and Cross Flow Conditions

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• Spray interaction with supersonic cross flows.
  – The applications can be found air breathing ramjet, scramjet and other supersonic engines, i.e., Pulse Detonation Engine.
  – There, Aerated injection is required for better penetration into high speed free stream while well maintaining the breakup.
  – So, such an aeration provides a well-mixed situation and thus, optimizes combustion performance.
• Focus of the theoretical modeling
  – CESE method
  – Gas phase governing equations
  – Stochastic Particle Solver in LS-DYNA

• Results
  – Initial conditions based on isentropic assumptions
  – Validation: spray penetrations and particle sizes
  – Spray flow
  – Close to near nozzle views
  – Flow field

• Concluding remarks
The CESE method is a high-resolution and genuinely multidimensional compressible flow solver for solving conservation laws using the Conservation Element/Solution Element method.

Unique features include:
- A unified treatment of space and time
- The introduction of the conservation element and the solution element as a vehicles for enforcing space-time flux conservation, locally and globally.
- A novel shock capturing strategy without a Riemann solver.
- Unlike conventional schemes, flow variables and their derivatives are solved simultaneously.
Euler vs. Navier-Stokes in CESE

- Euler equations:

\[
\begin{pmatrix}
\rho \\
\rho u \\
\rho v \\
\rho w \\
\rho E \\
\rho y_1 \\
\vdots \\
\rho y_n \\
\rho u \nu_j, \\
\rho y \nu_j
\end{pmatrix}
\begin{pmatrix}
\frac{\partial}{\partial t} \\
\frac{\partial}{\partial x} \\
\frac{\partial}{\partial y} \\
\frac{\partial}{\partial w} \\
\frac{\partial}{\partial E} \\
\frac{\partial}{\partial y_1} \\
\vdots \\
\frac{\partial}{\partial y_n} \\
\frac{\partial}{\partial u \nu_j} \\
\frac{\partial}{\partial y \nu_j}
\end{pmatrix}
\begin{pmatrix}
0 \\
0 \\
0 \\
0 \\
0 \\
0 \\
0 \\
0 \\
0 \\
0
\end{pmatrix}
\]

\[E = e + \frac{1}{2}(u^2 + v^2 + w^2), \quad p = p(\rho, e, y) = \rho R(y)T(e, y)\]

- N-S equations:

\[
\begin{pmatrix}
\rho \\
\rho u \\
\rho v \\
\rho w \\
\rho E \\
\rho y_1 \\
\vdots \\
\rho y_n \\
\rho u \nu_j, \\
\rho y \nu_j
\end{pmatrix}
\begin{pmatrix}
\frac{\partial}{\partial t} \\
\frac{\partial}{\partial x} \\
\frac{\partial}{\partial y} \\
\frac{\partial}{\partial w} \\
\frac{\partial}{\partial E} \\
\frac{\partial}{\partial y_1} \\
\vdots \\
\frac{\partial}{\partial y_n} \\
\frac{\partial}{\partial u \nu_j} \\
\frac{\partial}{\partial y \nu_j}
\end{pmatrix}
\begin{pmatrix}
0 \\
\tau_{xx} \\
\tau_{xy} \\
\tau_{xz} \\
\Phi_x \\
-\rho y_i \ddot{u}_i \\
\vdots \\
-\rho y_i \ddot{u}_n,
\end{pmatrix}
\]

\[\tau_{xx} = \frac{2\mu}{3Re}\left(2\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} - \frac{\partial w}{\partial z}\right), \quad \tau_{xy} = \frac{\mu}{Re}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right), \quad \tau_{xz} = \frac{\mu}{Re}\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right)\]

- Depending on viscous forces
  - Euler: small viscous effects
  - N-S: important viscous

- 2-D, 3-D, and fluid-structure interaction (FSI) capabilities
  - SMP
  - Parallel computing via MPI

\[\mu = \mu(T, y), \quad k = k(T, y), \quad D_{km} = D_{km}(T, y).\]

\[h_k : \text{the enthalpy of species } k, \quad y_k : \text{the mass fraction of species } k, \quad \ddot{u}_k : \text{the diffusion x-dir velocity of species } k\]
CESE coupling to spray solver

CESE chemistry and stochastic particle solver couplings

CESE
Explicit
Double precision

Source terms: density, momentum, energy
Density, velocity, Temperature, energy

Chemistry
Implicit reactions
& Explicit transport
Double precision

Stochastic
Particle Solver
Explicit
Double precision

Source terms: density, momentum, energy
Density, Temperature, Pressure

CESE chemistry and stochastic particle solver couplings
• Stochastic particle flow:
  – Theoretical background
  – Stochastic particle injection
  – Breakup models
  – Non-evaporating vs. evaporating sprays
• Stochastic particles or sprays:

The particles or spray drops can be represented by a certain probability distribution function as,

$$ f = f(x, V, r, T_d, y, y', t) $$

three droplet positions: $x$, three velocity components: $v$
equilibrium radius: $r$, temperature: $T_d$
distortion from sphericity: $y$, time rate of the distortion: $y'$
time: $t$

$$ \frac{\partial f}{\partial t} + \nabla_x \cdot (f \ V) + \nabla_v \cdot (f \ F) + \frac{\partial}{\partial r} (f \ r) + \frac{\partial}{\partial T_d} (f \ T) + \frac{\partial}{\partial r} (f y) + \frac{\partial}{\partial r} (f \ y') $$

$$ = \dot{f}_{\text{breakup}} + \dot{f}_{\text{collision}} $$
To simulate the complicate stochastic particles or sprays, the initial distribution of particles via injection is required.

- Mono – dispersed
  \[ f(r) = R, \ R: \text{const. radius} \]

- Rosin – Rammler
  \[ f(r) = 1 - \exp\left(-\frac{r^{3.5}}{\bar{r}}\right), \]
  \( \bar{r}: \text{average radius} \)

- \( \chi^2 \) – degree of 4
  \[ f(r) = \frac{r}{2\bar{r}^2} \exp\left(-\frac{r}{\bar{r}}\right), \]
  \( \bar{r}: \text{average radius} \)

- \( \chi^2 \) – degree of 2
  \[ f(r) = \frac{1}{\bar{r}} \exp\left(-\frac{r}{\bar{r}}\right), \]
  \( \bar{r}: \text{average radius} \)
• TAB model (SAE 872089):
  
  • Taylor’s analogy between an oscillating, distorting drop and a spring mass system.

  \[
  \ddot{y} = \frac{C_F}{C_B} \frac{\rho_g u^2}{\rho_l r^2} - \frac{C_s \sigma}{\rho_l r^3} y - \frac{C_d \mu_l}{\rho_l r^2} \ddot{y} \\
  y(t) = \frac{C_F}{C_k C_B} W_e + e^{-\gamma t} \left( y_o - \frac{C_F}{C_k C_B} W_e \right) \cos \omega t + \frac{1}{\omega} \left( \dot{y}_o + \frac{C_F}{C_k C_B} \frac{W_e}{t_d} \right) \sin \omega t \\
  W_e = \frac{\rho_g u^3 r}{\sigma}, \quad y_o = y(0), \quad \dot{y}_o = \frac{dy}{dt}(0), \quad \frac{1}{t_d} = \frac{C_d}{2} \frac{\mu_l}{\rho_l r^2}, \quad \omega^2 = C_k \frac{\sigma}{\rho_l r^3} - \frac{1}{t_d^2}
  \]

• Kelvin-Helmholtz/Rayleigh-Taylor hybrid model:

  • Breakup initiation time instead of breakup length.
  • Mass reduction rate: sinusoidal function.
  • Allowed secondary breakup (R-T) for a droplet generated by K-H mode.
Non-evaporating vs. evaporating spray flows

- **Non-evaporating spray:**

\[
\begin{aligned}
\frac{\partial}{\partial t} \begin{pmatrix}
\rho \\
\rho u \\
\rho v \\
\rho w \\
\rho E
\end{pmatrix} + \frac{\partial}{\partial x} \begin{pmatrix}
\rho u \\
\rho u^2 + p \\
\rho uv \\
\rho uw \\
(\rho E + p)u
\end{pmatrix} - \frac{\partial}{\partial x} \begin{pmatrix}
\tau_{xx} \\
\tau_{xy} \\
\tau_{xz} \\
\Phi_x \\
\theta
\end{pmatrix} + \cdots = \begin{pmatrix}
\dot{\rho}_s \\
(\dot{m}_s)_s \\
(\dot{m}_y)_s \\
(\dot{m}_z)_s \\
\dot{E}_s
\end{pmatrix}
\end{aligned}
\]

\[
E = e + \frac{1}{2}(u^2 + v^2 + w^2), \quad p = p(\rho, T) = \rho RT
\]

\[
\tau_{xx} = \frac{2\mu}{3\text{Re}} \left( 2 \frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} - \frac{\partial w}{\partial z} \right),
\]

\[
\tau_{xy} = \frac{\mu}{\text{Re}} \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right),
\]

\[
\tau_{xz} = \frac{\mu}{\text{Re}} \left( \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right),
\]

\[
\Phi_x = u\tau_{xx} + v\tau_{sy} + w\tau_{sz} + k \frac{\partial T}{\partial x}
\]

- **Evaporating spray:**

\[
\begin{aligned}
\frac{\partial}{\partial t} \begin{pmatrix}
\rho \\
\rho u \\
\rho v \\
\rho w \\
\rho E
\end{pmatrix} + \frac{\partial}{\partial x} \begin{pmatrix}
\rho u \\
\rho u^2 + p \\
\rho uv \\
\rho uw \\
(\rho E + p)u
\end{pmatrix} - \frac{\partial}{\partial x} \begin{pmatrix}
\tau_{xx} \\
\tau_{xy} \\
\tau_{xz} \\
\Phi_x \\
\theta
\end{pmatrix} + \cdots = \begin{pmatrix}
\dot{\rho}_s \\
(\dot{m}_s)_s \\
(\dot{m}_y)_s \\
(\dot{m}_z)_s \\
\dot{E}_s
\end{pmatrix}
\end{aligned}
\]

\[
E = e + \frac{1}{2}(u^2 + v^2 + w^2), \quad p = p(\rho, e, y) = \rho R(y)T(e, y)
\]

\[
\tau_{xx} = \frac{2\mu}{3\text{Re}} \left( 2 \frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} - \frac{\partial w}{\partial z} \right), \quad \tau_{xy} = \frac{\mu}{\text{Re}} \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right), \quad \tau_{xz} = \frac{\mu}{\text{Re}} \left( \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right)
\]

\[
\Phi_x = u\tau_{xx} + v\tau_{sy} + w\tau_{sz} + k \frac{\partial T}{\partial x} + \sum_{k=1}^{n} h_k \rho y_k \tilde{u}_k
\]

\[
y_k \tilde{u}_k = -D_{km} \frac{\partial y_k}{\partial x}
\]

\[
\mu = \mu(T, y), \quad k = k(T, y), \quad D_{km} = D_{km}(T, y),
\]

\[
h_k : \text{ the enthalpy of species } k \quad y_k : \text{ the mass fraction of species } k \quad \tilde{u}_k : \text{ the diffusion x-dir velocity of species } k
\]
Initial conditions for aerated injection

- **Choked condition at nozzle exit:**
  - Air velocity higher than sonic speed
  - Calculate the critical variables, $T^*$, and $\rho^*$
  - Use isentropic equations between inside nozzle and nozzle exit to calculate inside pressure
  - Apply isentropic equation to calculate critical pressure $P^*$

  \[
  \left( m_g \right)_{\text{in}} = 0.1276 \text{ g/s}, \quad \left( m_g \right)_{\text{out}} = 0.3190 \text{ g/s}
  \]

  Applying the choked condition at nozzle exit

  \[
  \left( m_g \right) = \rho^* A^* a^*, \quad a^* = \sqrt{\gamma RT^*}
  \]

  Get $\rho^*$, and $T^*$

  From isentropic relations,

  \[
  \frac{\rho_0}{\rho^*} = \left( 1 + \frac{\gamma - 1}{2} \right)^{1/(\gamma - 1)}; \quad \frac{T_0}{T^*} = \left( 1 + \frac{\gamma - 1}{2} M \right)
  \]

  Since $P_0 = \rho_0 RT_0$, we have $P_0$

  Finally, by using,

  \[
  \frac{P_0}{P^*} = \left( 1 + \frac{\gamma - 1}{2} \right)^{\gamma/(\gamma - 1)}
  \]

  Therefore, obtained initial conditions at nozzle exit

- **Inner diameter: 60% of the nozzle diameter:**
  - 60% of the nozzle diameter: $D_i/D_o = 60\%$
  - Based on X-ray experiment
Results – test cases with average calculations

• Supersonic cross flow at mach number 1.94:
  – Test section: 127 X 152 X 762 mm wind tunnel
  – Test liquid: standard water
  – Wind condition: total pressure and temperature: 206 kPa and 533 K
  – Corresponding static pressure and temperature: 29 kPa and 304 K
  – Velocity: 678.13 m/s

<table>
<thead>
<tr>
<th>Case</th>
<th>T₀ (K)</th>
<th>d₀ (mm)</th>
<th>x/d₀</th>
<th>q₀</th>
<th>GLR (%)</th>
<th>SMD (µm)</th>
<th>u_p/u_z (%)</th>
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<td>Simulated</td>
</tr>
<tr>
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<tr>
<td>A2</td>
<td>533</td>
<td>0.5</td>
<td>200</td>
<td>7</td>
<td>5</td>
<td>13.2</td>
<td>12.5</td>
</tr>
</tbody>
</table>
Results – Spray structure and validation

- Spray structure at Mach number 1.94:
  - Numerical simulation for the non-aerated case
  - Shadow graphic visualization

- Comparisons of the spray penetration heights:
  - Shadow, PDPA, and simulation

\[
\text{Shadow: } \frac{h_0}{d_0} = 3.94 \cdot q_0^{0.47} \left( \frac{x}{d_0} \right)^{0.21}
\]

\[
\text{PDPA: } \frac{h_0}{d_0} = 4.73 \cdot q_0^{0.30} \left( \frac{x}{d_0} \right)^{0.30}
\]
Results – Aerated sprays

- Spray structures: GLR=0, GLR=2%, and GLR=5%
Results – Penetration Heights

- Spray penetration heights
• Droplet size comparisons with experimental data:

• Droplet size comparisons between GLR=2% and 5%

• Droplet velocity comparisons between GIR=2% and GLR=5%
• Geometry partition using LS-PrePost software:
  - Free software
  - Download at www.lstc.com/product/ls-prepost
Results – Near nozzle views(2)

- Near nozzle views:
Spray results – Flow fields

- Flow field structure:
  - High speed free stream
  - Interacting with spray
  - Develop conical shock
  - Complex shock trains at down stream
A study of the numerical simulation for the spray analysis in the cross flow has been conducted with non-aerated and aerated liquid jets without and with GLR conditions.

- LS-DYNA CESE compressible solver was used to simulate a highly compressible flow in a supersonic wind tunnel.
- The spray penetration height was well validated with different diagnostics: shadow and PDPA measurement.
- The simulation results for the drop size were well agree with data.
- The effects of aeration on the spray penetration and atomization were explored, and found that the aerated injection is necessary for the spray to penetrate into a high speed free stream.
- Complex shock waves in the flow field were developed by interacting with the liquid jets.
• LSTC will continue to advance each of these solvers

• New features and algorithms will be continuously implemented to handle new challenges and applications:
  – Fluid-Structure-Spray interaction problems
  – Starting Eulerian and solving Euler-Lagrangian problems
  – Eulerian to Eulerian particle solver for dense particle flows
  – Coupling with more solvers in LS-DYNA
  – More turbulence models in the CESE solver
  – Spray & combustion via CESE chemistry solvers.

• Hybrid MPI/OPENMP developments are currently being pursued for accelerating the CESE, and stochastic particle solvers.
Thank You!