Numerical simulation of turbulent jet primary breakup in Diesel engines

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"Micro-Macro Modelling and Simulation of Liquid-Vapour Flows"  
Spray in Combustion Devices

- Fuel is typically injected as a liquid
- Combustion only in the gaseous phase
- Mixture composition pollutant formation
- Combustion stability
- Need to accurately model Spray Process
- From injection to evaporation
The Challenge of Modeling Spray

The Spray Model we have
- Empirical nature.
- wide range of Parameters.
- Experiments Calibration.

The Experiments are difficult
- complex Injection System.
- high Pressure.
- high Temperature.
- Fuel Properties.

Primary Breakup, the beginning of the spray, is particularly poorly understood.
Modeling Spray Primary Breakup

Modeling approach

- split into primary & secondary atomization
- track the complex phase interface geometry during primary breakup
- assume simple phase interface geometry for secondary breakup
- couple with secondary atomization models
DNS Diesel Injection done by Marcus

- Injector diameter: \( D = 100 \, \mu m \)
- Flow solver resolution: \( D/50 = 2.0 \, \mu m \)
- Level Set Solver resolution: \( D/64 = 1.56 \, \mu m \)
- Injection Velocity: 100 m/s
- Inlet profile: DNS of \( \text{Re}=5000 \) turbulent pipe
- Density ratio: 850/25
- Viscosity ratio: \( 1.70E-3/1.78E-5 \)
- Surface tension coefficient: 0.05 N/m

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DNS Diesel Injection Results

Time = 6.901

Time = 7.001

Time = 7.100

Time = 7.302
DNS Diesel Injection Results

Drop velocity PDF

Drop size PDF
The Governing Equations

Navier-Stokes

\[ \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \frac{1}{\rho} \nabla \cdot (\mu(\nabla \mathbf{u} + \nabla^T \mathbf{u})) + \mathbf{g} + \frac{1}{\rho} \mathbf{T}_\sigma \]
\[ \nabla \cdot \mathbf{u} = 0 \]

Level-Set

\[ \frac{\partial G}{\partial t} + \mathbf{u} \cdot \nabla G = 0 \]

VOF Modification

\[ \rho = \psi \rho_1 + (1 - \psi) \rho_2 \]
\[ \mu = \psi \mu_1 + (1 - \psi) \mu_2 \]

Surface Tension Force

\[ \mathbf{T}_\sigma(\mathbf{x}) = \sigma \kappa \delta(\mathbf{x} - \mathbf{x}_f) \mathbf{n} \]
\[ \mathbf{n} = \frac{\nabla G}{|\nabla G|}, \quad \kappa = \nabla \cdot \mathbf{n} \]
Numerics and Performances of two-phase flow solver

Unstructured, Collocated, Finite volume Navier-Stokes Solver

\[ \partial_t u + \bar{u} \partial_x u - \partial_{xx} u / Re = 0 \]

\[ M \frac{d\mathbf{u}}{dt} + C(\bar{u})\mathbf{u} + D\mathbf{u} = 0 \]

for \( D = 0 \), Energy \( \| \mathbf{u} \|^2 = \mathbf{u}^* M \mathbf{u} \) is conserved if and only if
\[ \frac{d}{dt} \| \mathbf{u} \|^2 = -\mathbf{u}^* (C(\bar{u}) + C^*(\bar{u})) \mathbf{u} = 0 \]

- Skew-symmetry of convective derivative: \( C(\bar{u}) + C^*(\bar{u}) = 0 \)
- Symmetric, positive-definite diffusive operator
- DNS \( \Leftrightarrow \) do not want numerical dissipation!
Numerics and Performances of two-phase flow solver

Refined Level Set Grid Method

- Introduce equidistant Cartesian super-grid (blocks)
- Activate (store) only narrow band of blocks
- Active blocks consist of an equi-distant Cartesian fine G-grid
- Activate (store) only narrow band of fine G-grid

⇒ Advantages: low cost of storage, efficient domain decomposition, straightforward parallelization, fast and accurate cartesian solution methods (5th order WENO, FMM)
Phase Transition Diagram

**Liquid Phase**

**Without Phase Transition**

**With Phase Transition**

**Gaseous Phase**

**Without Phase Transition**

**With Phase Transition**
Phase Transition Models

Introduce a **Surface Regression Velocity** $s_P$

### New Term in Navier-Stokes

\[
\frac{\partial \bm{u}}{\partial t} + \bm{u} \cdot \nabla \bm{u} = -\frac{1}{\rho} \nabla p + \bm{g} + \frac{1}{\rho} \bm{T}_\sigma \\
+ \frac{1}{\rho} \nabla \cdot (\mu(\nabla \bm{u} + \nabla^T \bm{u})) + \frac{1}{\rho} \bm{T}_p
\]

where $\bm{T}_p$ is the balance force for evaporation.

\[
\bm{T}_p = (\rho_1 - \rho_2)s_P \delta(x - x_f) \bm{u}
\]

$\delta$ is the delta-function.

### New Term in Level-Set

**phase interface**

\[
\frac{dx_f}{dt} = \bm{u} + s_P \bm{n},
\]

\[
\frac{\partial G}{\partial t} + \bm{u} \cdot \nabla G + s_P |\nabla G| = 0
\]
G field of evaporating Droplet
Numerics for Balance Force Term

Predictor

\[
\rho_{c}^{n+1} \mathbf{u}_{c}^{*} = \rho_{c}^{n} \mathbf{u}_{c}^{n} - \Delta t \sum_{f} \mathbf{u}_{c}^{n} \left( \sum_{k} \rho_{k} f_{k} \right) (\mathbf{u}_{f} \cdot \mathbf{n}_{f}) A_{f}
\]

\[
- \Delta t \rho_{c}^{n+1} \left\langle \frac{\nabla P}{\rho_{f}} - \frac{T_{f}}{\rho_{f}} \right\rangle_{f \rightarrow c}^{n}
\]

(1)

Projection

\[
\mathbf{u}_{f}^{*} = \left\langle \mathbf{u}_{c}^{*} + \Delta t \left\langle \frac{(\nabla P)_{f}}{\rho_{f}} - \frac{T_{f}}{\rho_{f}} \right\rangle_{t \rightarrow c}^{n} \right\rangle_{c \rightarrow f} - \frac{\Delta t}{\rho_{f}^{n+1}} [((\nabla P)_{f}^{n} - T_{f}^{n+1})]
\]

(2)

Corrector

\[
\nabla \cdot \left( \frac{(\nabla \delta P_{c}^{n+1})_{f}}{\rho_{f}^{n+1}} \right) = - \nabla \cdot \left( \frac{\mathbf{u}_{f}^{*}}{\Delta t} \right).
\]

(3)

\[
\mathbf{u}_{f}^{n+1} = \mathbf{u}_{f}^{*} - \Delta t \left( \frac{(\nabla \delta P_{c}^{n+1})_{f}}{\rho_{f}^{n+1}} \right),
\]

(4)

\[
\mathbf{u}_{c}^{n+1} = \mathbf{u}_{c}^{*} + \Delta t \left\langle \frac{(\nabla P)_{f} - T_{f}}{\rho_{f}} \right\rangle_{f \rightarrow c}^{n} - \Delta t \left\langle \frac{(\nabla P)_{f} - T_{f}}{\rho_{f}} \right\rangle_{f \rightarrow c}^{n+1}
\]

(5)
Stability Analysis of Phase Transition

Equation of Perturbation Motion

\[ \nabla \cdot \mathbf{u}' = 0, \quad \partial \mathbf{u}' / \partial t + \mathbf{u} \cdot \nabla \mathbf{u}' = -1 / \rho \nabla p' \]

Boundary Conditions

\[ p'_1 - p'_2 = s_L (\rho_1 - \rho_2) \zeta (y, t), \]
\[ u'_1 - \partial \zeta / \partial t = u'_2 - \partial \zeta / \partial t, \]
\[ v'_1 + v_1 \partial \zeta / \partial t = v'_2 + v_2 \partial \zeta / \partial t \]

Particular Solution

\[ u'_1 = A e^{i k y + k x - i \omega t} \]
\[ u'_2 = B e^{i k y + k x - i \omega t} + C e^{i k y - i \omega t + i \omega x / v_2} \]
\[ \zeta = D e^{i k y - i \omega t} \]

Charac. Equation for Nontrivial Solution

\[
\begin{vmatrix}
\omega & -1 & 0 & 0 \\
\omega & 0 & 1 & \frac{i k v_2}{\epsilon k v_2} \\
0 & 1 + \frac{i \omega}{\epsilon k v_2} & 1 + \frac{i \omega}{k v_2} & \frac{2 \mu}{\omega k v_2} \\
- i k (\epsilon - 1) v_2 & 1 & -1 & -1
\end{vmatrix} = 0
\]

Result

\[ \epsilon = \rho_2 / \rho_1 < 1 \]
\[ \omega \text{ has positive imaginary part} \]
\[ - i \omega = - \epsilon + \epsilon \sqrt{1 - \epsilon + \epsilon^{-1}} v_2 k \]

The evaporation front is unstable.
Rayleigh-Taylor Instability
Comparison of DNS, LES and RANS

**DNS**

\[ u(x, t) \]

**LES**

\[ u(x, t) = \bar{u} + u' \]
\[ \bar{u}(x, t) = \int \int \int G(\xi - x)u(\xi, t)d\xi \]

**RANS**

\[ u(x, t) = \bar{u} + u' \]
\[ \bar{u}(x, t) = \lim_{T \to \infty} \frac{1}{T} \int_0^T u(x, t)dt \]

**LES Equations**

\[ \frac{\partial \bar{u}_i}{\partial t} + \frac{\partial \bar{u}_i \bar{u}_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} + \frac{\tau_{ij}}{\partial x_j} \]

subgrid stress model \( \tau_{ij} = 2\mu_T S_{ij} \),

where \( S_{ij} = \frac{1}{2} \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \),

Smagorinsky eddy viscosity \( \mu_T = \rho(C_s\Delta)^2 \sqrt{S_{ij}S_{ij}} \),

Smagorinsky coefficient \( 0.10 < C_s < 0.24 \)
Energy Cascade

Energy dissipation rate modeled as $\varepsilon \sim \frac{u^2}{t} \sim \frac{u^3}{l} \sim \frac{l^2}{t^3}$

Kolmogorov Scales (Smallest)

- length $\eta \equiv \left(\frac{\nu^3}{\varepsilon}\right)^{1/4}$
- time $\tau_\eta \equiv \left(\frac{\nu}{\varepsilon}\right)^{1/2}$
- velocity $u_\eta \equiv \left(\nu \varepsilon\right)^{1/4}$

Ratio of Smallest/Largest

- $\eta/l_0 \sim Re^{-3/4}$
- $\tau_\eta/\tau_0 \sim Re^{-1/2}$
- $u_\eta/u_0 \sim Re^{-1/4}$

Kolmogorov’s hypothesis

At sufficiently high Reynolds number, the small-scale turbulent motion are statistically isotropic.

Instead of running 3D full scale DNS, we can test our model on isotropic turbulent environment.
DNS of Isotropic Turbulence in Cubic Box

- Grid: $128^3 \sim 2$ Million
- Boundary Condition
  - Periodic in all directions
- Initial Condition
  - $Re_\lambda = 120 \sim 200$
- Some Numerics
  - time: Crank-Nicolson
  - spatial: Skew-sym. Con.
  - staggered $p$ and $u$
  - predictor-corrector
  - preconditioner: Hypre
- Parallelization
  - Domain-decomposition: ParMetis
  - Parallel I/O

Turbulent Energy is decaying!
Linear forced turbulence

**Theory**

\[
\frac{\partial u}{\partial t} + u \cdot \nabla u = -\nabla p/\rho + \nu \nabla^2 u + f
\]

\[
f = Qu \quad \text{where} \quad Q = \epsilon/3U^2,
\]

\[
\epsilon = -\nu \nabla \cdot \nabla^2 u,
\]

\[
U^2 = \langle u \cdot u \rangle / 3
\]

<table>
<thead>
<tr>
<th>CDP variable</th>
<th>Description</th>
<th>set in Subroutine</th>
</tr>
</thead>
<tbody>
<tr>
<td>Q</td>
<td>$Q : \text{scalar for linear forcing}$</td>
<td>momentum_source_hook</td>
</tr>
<tr>
<td>epsilon</td>
<td>$\epsilon : \text{mean dissipation rate}$</td>
<td>momentum_source_hook</td>
</tr>
<tr>
<td>UU</td>
<td>$3U^2 : \text{velocity square}$</td>
<td>momentum_source_hook</td>
</tr>
</tbody>
</table>

**Table**: New Variables

**F90 implementation**

```
do icv = 1, gp%ncv_ib
    UU = dot_product(ifp%u(1:3,icv),ifp%u(1:3,icv))
```
Phase Interface
Summary

- DNS for Spray Primary Breakup
- Introduce $s_P$ for Phase Transition Modeling

Outlook

- Terabyte DNS
- Modeling Approach
- Cavitation
For Further Reading

Norbert Peters.  
*Turbulent Combustion.*  

Marcus Herrmann.  
A balanced forced Refined Level Set Grid method for two-phase flows on unstructured flow solver grids.  