Modeling of Diesel Fuel Spray Formation in OpenFOAM

Anne Kösters (Chalmers Univ of Technology)
Anders Karlsson (Volvo Technology Corporation)
Motivation

- Sprays are involved in many applications
  (internal combustion engines, exhaust aftertreatment, gas turbines...)
- CFD is an increasingly used tool in the development of these applications
- Spray and combustion models include many sub models
- Numerical unrobustness & many tuning parameters is an issue
Spray phenomena

- breakup
- evaporation and heat transfer
- droplet drag
- spray induced turbulence
- combustion
parcels
Spray Modeling - Shortcomings

McKinley & Primus*

“cell widths are large and […] inadequate for capturing the strong gradients in velocity, temperature and fuel vapor concentration. This leads to under prediction of gas velocities and over prediction of gas temperatures within the spray”

- Grid dependence
- Time step dependence
- Robustness
- Tuning parameters (sub models)

Work that has been done

McKinley, T.L. & Primus, R.J., ASME paper 90-ICE-2
Abraham, J., SAE technical paper 970051
Wan, Y.P. & Peters, N., SAE technical paper 972866
Abraham, J. & Magi, V., SAE technical paper 1999-01-0911
Durand, P et. al, SAE technical paper 960632
SAE technical paper 980134

Bédard et. al, SAE 2000-01-1893
(CLE: “Couplage Lagrangien-Eulérien)

- Gaseous drop

Abani et. al, SAE 2008-01-0970

- Gas jet theory used for gas velocity

\[
\nu_x = \nu_{gas} = \frac{m_t n}{U_{inj}} \left[ \frac{3U_{inj}^2 d_{eq}^2}{32\nu_t x \left( 1 + \frac{3U_{inj}^2 d_{eq}^2 r^2}{256\nu_t^2 x^2} \right)^2} \right]
\]
VSB2 Spray Model

Vsb2 stochastic Blob and Bubble model

- Unconditional robust
- Minimal number of parameters
- Adaptable to any CFD code feat. particle tracking

*developed by Karlsson, A. (Volvo Tech. Corp.)

results using OpenFOAM code are published in:

results using STAR-CD code are published in:
Husberg, T., Denbratt, I. and Karlsson, A., SAE 2008- 01-1328
Eismark, J. et al., presented at Thiesel 2010, Valencia
Standard spray model

**parcel**

collection of equal droplets

E.g. consider the energy balance of the parcel:

\[
m_d \frac{dh_d}{dt} = \pi D_d k(T_g - T_d) f(z) Nu + h_v \frac{dm_d}{dt}
\]

Problem: How can \(T_g\) be estimated if there are more than one parcel within the cell and/or there is a high evaporation rate?
VSB2 spray model – blob

**parcel**
collection of equal droplets

**blob**
droplet size distribution (based on local instantaneous We and Oh), using break-up rate correlations by Pilch & Erdman*

VSB2 spray model – blob

E.g. gas phase enthalpy source

\[ m_b \Delta h_b = \sum_{i=1}^{10} m_{b,i} \Delta h_{b,i} \]
VSB2 spray model – bubble

**Common spray model**

Gas phase in one **cell** used to calculate the interaction with the parcel

**VSB2 spray model**

Gas phase in a **bubble** used to calculate the interaction with the blob

\[
V_{bub} = \frac{\pi}{6} N_D \left[ (D_B + l_t)^3 - D_B^3 \right]
\]

\[
l_t = \min \left[ \frac{k^{3/2}}{C \epsilon}, V_{cell}^{1/3} \right]
\]
VSB2 spray model – robustness

Relaxation equations (based on equilibrium)

<table>
<thead>
<tr>
<th></th>
<th>( \frac{dU_{j,b,i}}{dt} = \frac{U_{eq} - U_{j,b,i}}{\tau_U} )</th>
<th>( \tau_U = \frac{4 \rho_b D_b}{3 \rho C_D U_R} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>mass</td>
<td>( \frac{dm_{b,i}}{dt} = \frac{m_{eq} - m_{b,i}}{\tau_m} )</td>
<td>( \tau_m = \frac{\rho_b D_b^2 R T_{m}}{6D Sh p} )</td>
</tr>
<tr>
<td>energy</td>
<td>( \frac{dT_{b,i}}{dt} = \frac{T_{eq} - T_{b,i}}{\tau_T} )</td>
<td>( \tau_T = \frac{\rho_b D_b^2 C_{p,b}}{6k f(z) Nu} )</td>
</tr>
</tbody>
</table>

Anne Kösters

CFD simulation of I.C. engines using OpenFOAM, Milano, 2011/07/11
VSB2 spray model – equilibrium

Momentum: \[ U_{j,eq} = \frac{\left( \rho V_{bub} U_{j,bub} + m_b U_{j,b} \right)}{\left( \rho V_{bub} + m_b \right)} \]

Mass & energy:

1. **Mass**: evaporation → saturation (incl. heat of vaporization)
   → \( m_{eq} \) is remaining blob mass

2. **Heat**: \( T_{eq} \) calculated after evaporation
Modifications in the *dieselSpray* library:

<table>
<thead>
<tr>
<th>parcel</th>
<th>rewritten</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>spraySubModels</strong></td>
<td></td>
</tr>
<tr>
<td>atomizationModel</td>
<td>atomizationModel</td>
</tr>
<tr>
<td>heatTransferModel</td>
<td>heatTransferModel</td>
</tr>
<tr>
<td>breakupModel</td>
<td>breakupModel</td>
</tr>
<tr>
<td>injectorModel</td>
<td>injectorModel</td>
</tr>
<tr>
<td>collisionModel</td>
<td>collisionModel</td>
</tr>
<tr>
<td>wallModel</td>
<td>wallModel</td>
</tr>
<tr>
<td>dispersionModel</td>
<td>dispersionModel</td>
</tr>
<tr>
<td>dragModel</td>
<td>dragModel</td>
</tr>
<tr>
<td>evaporationModel</td>
<td>evaporationModel</td>
</tr>
</tbody>
</table>
Numerical Set-up

- fuel: n-hexadecane
- tuned k-ε model (C₁ & σₐε)

Injector position:

Default grid in all simulations:

0.5x0.5x1.0 mm
232 320 cells
Results
(SAE 2011-01-0842)

Experiments:
Siebers & Naber
(SAE 960034, SAE 980809)

\(p_{\text{gas}} = 19.5 \text{ bar}\)

\(p_{\text{gas}} = 168 \text{ bar}\)

\(p_{\text{gas}} = 40 \text{ bar}\)

Anne Kösters
CFD simulation of I.C. engines using OpenFOAM, Milano, 2011/07/11
Definition of liquid penetration

$p_{gas} = 19.5 \text{ bar}$

Anne Kösters
CFD simulation of I.C. engines using OpenFOAM, Milano, 2011/07/11
Chalmers HP/ HT spray rig*  
(SAE 2011-01-0842)

$p_{\text{gas}} = 30 \text{ bar}$  
$T = 500^\circ \text{C}$

$p_{\text{gas}} = 50 \text{ bar}$  
$T = 410^\circ \text{C}$

$p_{\text{gas}} = 70 \text{ bar}$  
$T = 330^\circ \text{C}$

$p_{\text{gas}} = 70 \text{ bar}$  
$T = 500^\circ \text{C}$

Vapor & liquid penetration are indistinguishable

*experiments by Raúl Ochoterena, Chalmers University of Technology
Chalmers HP/HT spray rig*

(SAE 2011-01-0842)

\[ P_{\text{inj}} = 1200 \text{ bar} \]

\[ p_{\text{gas}} = 30 \text{ bar} \quad T = 500 \degree \text{C} \]

\[ p_{\text{gas}} = 50 \text{ bar} \quad T = 410 \degree \text{C} \]

\[ p_{\text{gas}} = 70 \text{ bar} \quad T = 330 \degree \text{C} \]

\[ p_{\text{gas}} = 70 \text{ bar} \quad T = 500 \degree \text{C} \]

*experiments by Raúl Ochoterena, Chalmers University of Technology*
Chalmers HP/HT spray rig, spray shape

(SAE 2011-01-0842)

Exp: Shadowgraphs
Sim: Temperature

\[ P_{\text{inj}} = 1200 \text{ bar} \]
\[ T_{\text{gas}} = 683 \text{ K} \]
\[ p_{\text{gas}} = 50 \text{ bar} \]

\( t = 0.4 \text{ ms} \)
\( t = 0.9 \text{ ms} \)
\( t = 1.4 \text{ ms} \)
\( t = 1.9 \text{ ms} \)

Anne Kösters
CFD simulation of I.C. engines using OpenFOAM, Milano, 2011/07/11
Discussion

- Robustness ++
- Tuning parameters ++
  (sub models)
Discussion

- Time step dependence +
- Robustness + +
- Tuning parameters + +

(sub models)

\( p_{\text{gas}} = 40 \) bar

![Graph showing time step dependency](image)
Discussion

- Grid dependence
- Time step dependence +
- Robustness + +
- Tuning parameters + +

(grid dependency, tip case rho14)

(exp, grid 0.5, grid 1.0, grid 1.5, grid 0.5, grid 1.0, grid 1.5, exp)

$\rho_{gas} = 40 \text{ bar}$

 penetration [mm]

0 20 40 60 80 100 120 140

0 0.5 1 1.5 2

time [ms]
Conclusions

- VSB2 spray model was successfully implemented in OpenFOAM
- VSB2 spray model combined with a tuned k-ε model predicts vapor and liquid penetration well under all tested conditions
- Robust!

Ongoing Work

- Combustion
  (Modification of Partially Stirred Reactor (PaSR model))
Thank you for your attention!

Anne Kösters
anne.kosters@chalmers.se