Numerical simulation of turbulent jet primary breakup in Diesel engines

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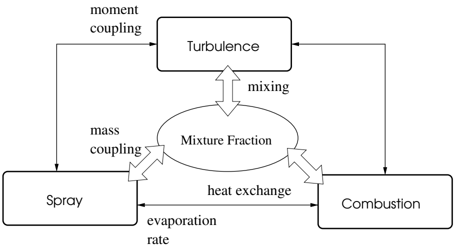
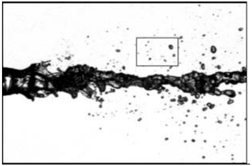
Outline

Motivation





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

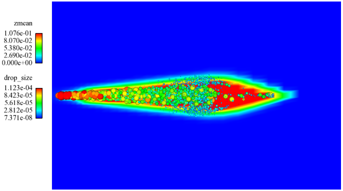
The Spray Model we have

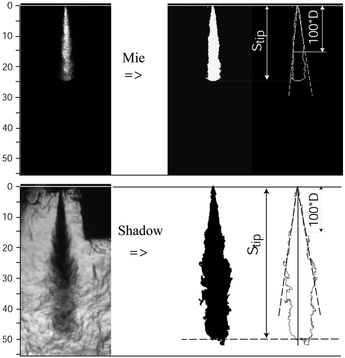
- Empirical nature.
- wide range of Parameters.
- Experiments Calibration.

The Experiments are difficult

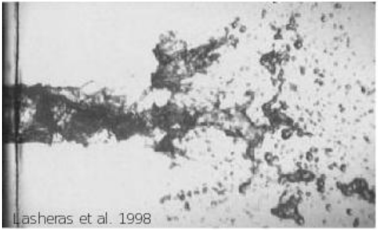
- complex Injection System.
- high Pressure.
- high Temperature.
- Fuel Properties.

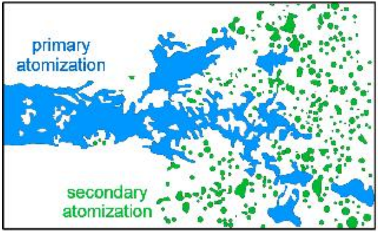
Primary Breakup, the beginning of the spray, is particularly poorly understood.





Modeling Spray Primary Breakup



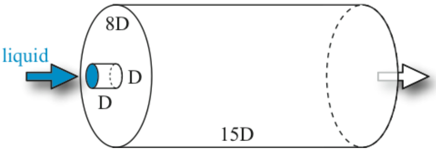


Modeling approach

- 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 μm
- Flow solver resolution :
  D/50 = 2.0 μm
- Level Set Solver resolution:
  D/64 = 1.56 μm
- Injection Velocity: 100 m/s
- Inlet profile: DNS of
  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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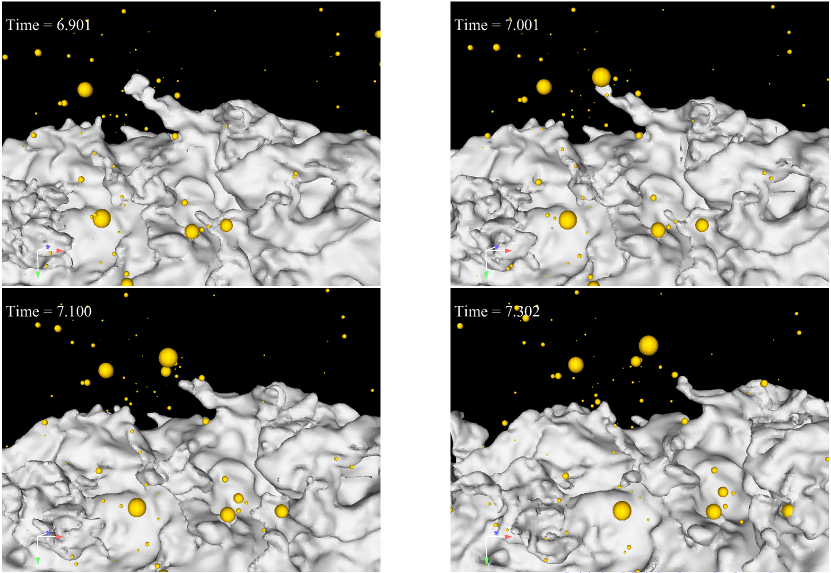
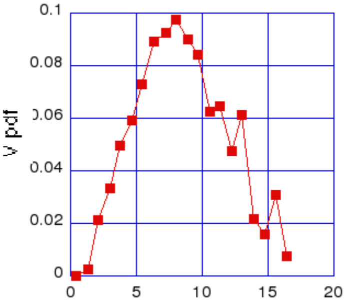
DNS Diesel Injection Results

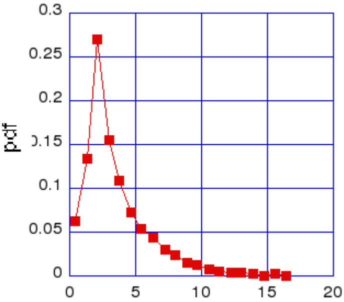


DNS Diesel Injection Results

Drop velocity PDF



Drop size PDF



The Governing Equations

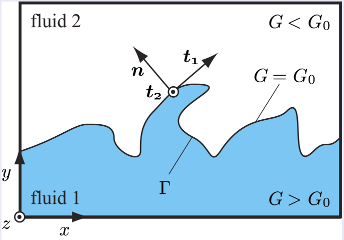
Navier-Stokes

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} = -\frac{1}{\rho}\nabla p + \frac{1}{\rho}\nabla \cdot (\mu(\nabla \boldsymbol{u} + \nabla^T \boldsymbol{u})) + \boldsymbol{g} + \frac{1}{\rho}\boldsymbol{T}_\sigma$$

$$\nabla \cdot \boldsymbol{u} = 0$$

Level-Set

$$\frac{\partial G}{\partial t} + \boldsymbol{u} \cdot \nabla G = 0$$



VOF Modification

$$\rho = \psi\rho_1 + (1 - \psi)\rho_2$$

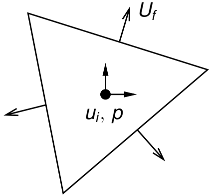
$$\mu = \psi\mu_1 + (1 - \psi)\mu_2$$

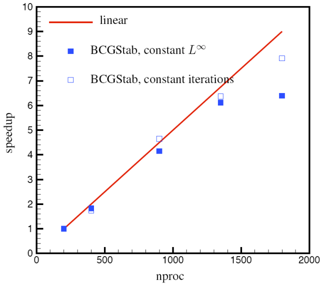
Surface Tension Force

$$\boldsymbol{T}_\sigma(\boldsymbol{x}) = \sigma\kappa\delta(\boldsymbol{x} - \boldsymbol{x}_f)\boldsymbol{n}$$

$$\boldsymbol{n} = \frac{\nabla G}{|\nabla G|}, \quad \kappa = \nabla \cdot \boldsymbol{n}$$

Numerics and Performances of two-phase flow solver





Unstructured, Collocated, Finite volume Navier-Stokes Solver

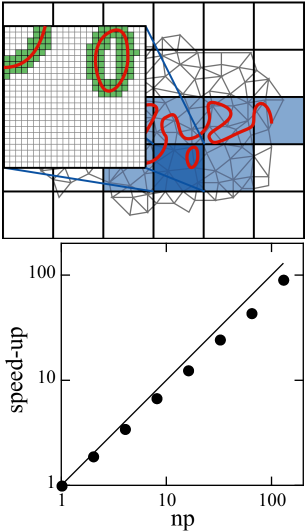
$$\partial_t u + \overline{u}\partial_x u - \partial_{xx} u / Re = 0$$

$$\boldsymbol{M}\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} + \boldsymbol{C}(\overline{u})\boldsymbol{u} + \boldsymbol{D}\boldsymbol{u} = 0$$

for $\boldsymbol{D} = 0$, Energy $\|\boldsymbol{u}\|^2 = \boldsymbol{u}^*\boldsymbol{M}\boldsymbol{u}$ is conserved if and only if $\frac{\mathrm{d}}{\mathrm{d}t}\|\boldsymbol{u}\|^2 = -\boldsymbol{u}^*(\boldsymbol{C}(\overline{u}) + \boldsymbol{C}^*(\overline{u}))\boldsymbol{u} = 0$

- Skew-symmetry of convective derivative : $\boldsymbol{C}(\overline{u}) + \boldsymbol{C}^*(\overline{u}) = 0$
- 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

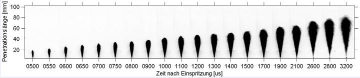
- Introduce equidistant Cartesian super-grid (blocks)
- Activate (store) only narrow band of blocks
- Active blocks consist of an equi-distant Cartesian fine G-grid
- Activate (store) only narrow band of fine G-grid

$\Rightarrow$ Advantages: low cost of storage, efficient domain decomposition, straightforward parallelization, fast and accurate cartesian solution mothods (5th order WENO, FMM)

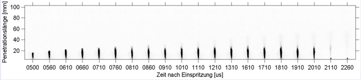
Phase Transition Diagram

Liquid Phase

Without Phase Transition

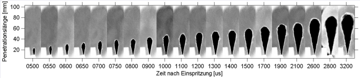


With Phase Transition

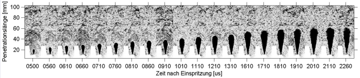


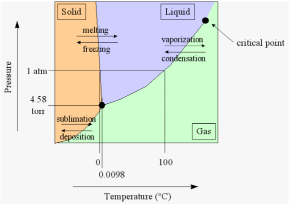
Gaseous Phase

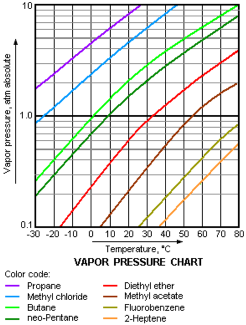
Without Phase Transition



With Phase Transition







Phase Transition Models

Introduce a **Surface Regression Velocity** s_P

New Term in Navier-Stokes

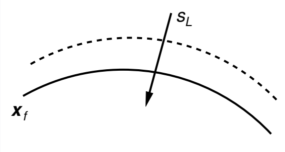
$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} = -\frac{1}{\rho}\nabla p + \boldsymbol{g} + \frac{1}{\rho}\boldsymbol{T}_\sigma + \frac{1}{\rho}\nabla \cdot (\mu(\nabla \boldsymbol{u} + \nabla^T \boldsymbol{u})) + \frac{1}{\rho}\boldsymbol{T}_p$$

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

$$\boldsymbol{T}_p = (\rho_1 - \rho_2) s_P \delta(\boldsymbol{x} - \boldsymbol{x}_f)\boldsymbol{u}$$

δ is the delta-function.

New Term in Level-Set

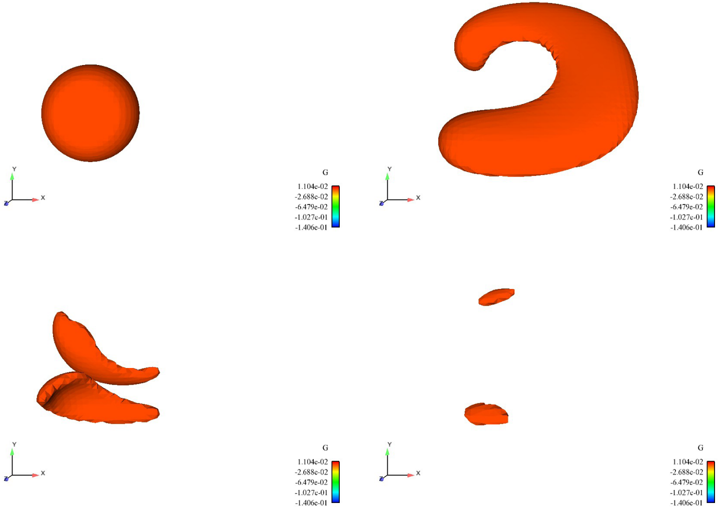


phase interface

$$\frac{d\boldsymbol{x}_f}{dt} = \boldsymbol{u} + s_P \boldsymbol{n},$$

$$\frac{\partial G}{\partial t} + \boldsymbol{u} \cdot \nabla G + s_P |\nabla G| = 0$$

G field of evaporating Droplet



Numerics for Balance Force Term

Predictor

$$\rho_c^{n+1}\boldsymbol{u}_c^{*} = \rho_c^{n}\boldsymbol{u}_c^{n} - \Delta t \sum_f \boldsymbol{u}_c^{n}\left(\sum_k \rho_k f_k\right)(\boldsymbol{u}_f \cdot \boldsymbol{n}_f)A_f - \Delta t \rho_c^{n+1}\left\langle \frac{\nabla P}{\rho_f} - \frac{\boldsymbol{T}_f}{\rho_f}\right\rangle_{f\to c}^{n} \quad (1)$$

Projection

$$\boldsymbol{u}_f^{*} = \left\langle \boldsymbol{u}_c^{*} + \Delta t \left\langle \frac{(\nabla P)_f}{\rho_f} - \frac{\boldsymbol{T}_f}{\rho_f}\right\rangle_{f\to c}^{n}\right\rangle_{c\to f} - \frac{\Delta t}{\rho_f^{n+1}}\left[(\nabla P)_f^{n} - \boldsymbol{T}_f{}^{n+1}\right] \quad (2)$$

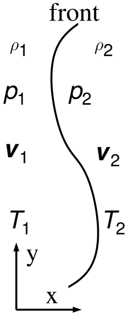
Corrector

$$\nabla \cdot \left(\frac{(\nabla \delta P_c^{n+1})_f}{\rho_f^{n+1}}\right) = -\nabla \cdot \left(\frac{\boldsymbol{u}_f^{*}}{\Delta t}\right). \quad (3)$$

$$\boldsymbol{u}_f^{n+1} = \boldsymbol{u}_f^{*} - \Delta t \left(\frac{(\nabla \delta P_c^{n+1})_f}{\rho_f^{n+1}}\right), \quad (4)$$

$$\boldsymbol{u}_c^{n+1} = \boldsymbol{u}_c^{*} + \Delta t \left\langle \frac{(\nabla P)_f - \boldsymbol{T}_f}{\rho_f}\right\rangle_{f\to c}^{n} - \Delta t \left\langle \frac{(\nabla P)_f - \boldsymbol{T}_f}{\rho_f}\right\rangle_{f\to c}^{n+1} \quad (5)$$

Stability Analysis of Phase Transition



Equation of Perturbation Motion

$$\nabla \cdot \boldsymbol{u}' = 0 \ , \ \partial \boldsymbol{u}'/\partial t + \boldsymbol{u} \cdot \nabla \boldsymbol{u}' = -1/\rho \nabla p'$$

Boundary Conditons

$$p_1' - p_2' = s_L(\rho_1 - \rho_2)\zeta(y,t),$$
$$u_1' - \partial\zeta/\partial t = u_2' - \partial\zeta/\partial t,$$
$$v_1' + v_1 \partial\zeta/\partial t = v_2' + v_2 \partial\zeta/\partial t$$

Particular Solution

$$u_1' = Ae^{iky+kx-i\omega t}$$
$$u_2' = Be^{iky+kx-i\omega t} + Ce^{iky-i\omega t+i\omega x/v_2}$$
$$\zeta = De^{iky-i\omega t}$$

Charac. Equation for Nontrivial Solution

$$\begin{vmatrix} \omega & -1 & 0 & 0 \\ \omega & 0 & 1 & \frac{ikv_2}{\omega} \\ 0 & 1+\frac{i\omega}{\epsilon k v_2} & 1+\frac{i\omega}{kv_2} & \frac{2ikv_2}{\omega} \\ ik(\epsilon-1)v_2 & 1 & -1 & -1 \end{vmatrix} = 0$$

Result

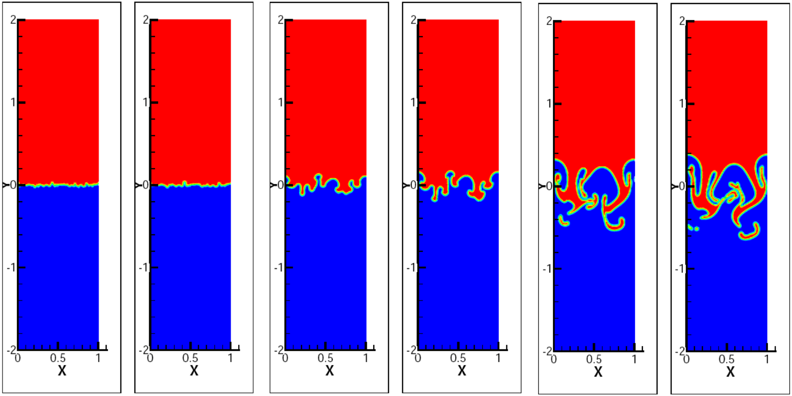
$\epsilon = \rho_2/\rho_1 < 1$

ω has positive imaginary part

$$-i\omega = \frac{-\epsilon+\epsilon\sqrt{1-\epsilon+\epsilon^{-1}}}{1+\epsilon} v_2 k$$

The evaporation front is unstable.

Rayleigh-Taylor Instability



Comparison of DNS, LES and RANS

DNS

$$u(\boldsymbol{x}, t)$$

LES

$$u(\boldsymbol{x}, t) = \overline{u} + u'$$

$$\overline{u}(\boldsymbol{x}, t) = \iiint G(\xi - \boldsymbol{x}) u(\xi, t) d\xi$$

RANS

$$u(\boldsymbol{x}, t) = \overline{u} + u'$$

$$\overline{u}(\boldsymbol{x}, t) = \lim_{T \to \infty} \frac{1}{T} \int_0^T u(\boldsymbol{x}, t) dt$$

LES Equations

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

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

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

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

Smagorinsky coeffcient $0.10 < C_s < 0.24$

Background Information

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

Ratio of Smallest/Largest

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

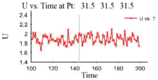
Kolmogorov's hypothesis

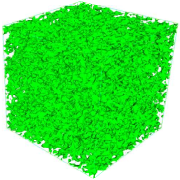
At sufficiently high Reynolds number, the small-scale turbulent motion are statistically isotropic.

Instead of running 3D full scale DNS, we can test our model on isotropic turbulent environment.

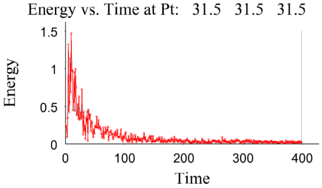
DNS of Isotropic Turbulence in Cubic Box

- 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-decompostion: ParMetis
  - Parallel I/O





Turbulent Energy is decaying!

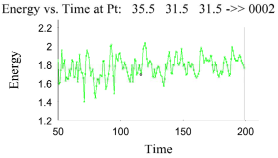


Linear forced turbulence

Theory

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

$\boldsymbol{f} = Q\boldsymbol{u}$ where $Q = \epsilon / 3U^2$,
$\epsilon = -\nu < \boldsymbol{u} \cdot \nabla^2 \boldsymbol{u} >$,
$U^2 = < \boldsymbol{u} \cdot \boldsymbol{u} > /3$



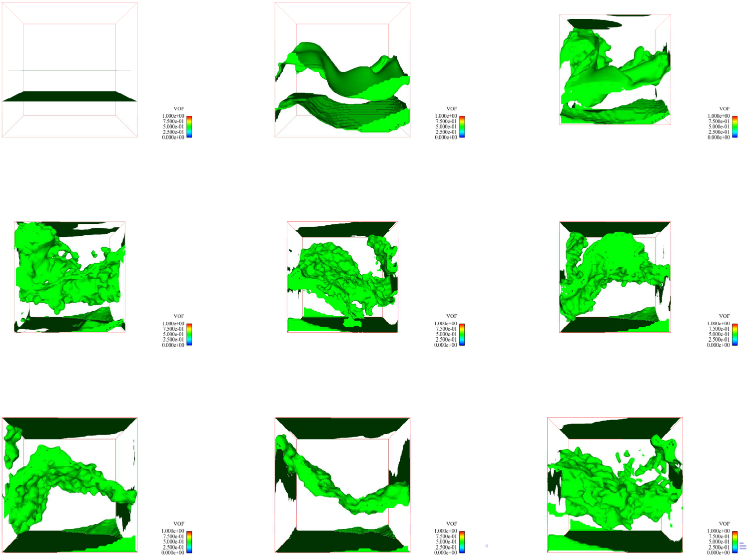
CDP variable	Description	set in Subroutine
Q	Q : scalar for linear forcing	momentum_source_hook
epsilon	ϵ : mean dissipation rate	momentum_source_hook
UU	$3U^2$: velocity square	momentum_source_hook

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.
Cambridge University Press, 2000.

Marcus Herrmann.
A balanced forced Refined Level Set Grid method for two-phase flows on unstructured flow solver grids.
Journal of Computational Physics, In Press, Accepted Manuscript, Available online 17 November 2007.