Direct Quadrature-based Sectional Method of Moments coupled to realistic evaporation models

Advanced Hybrid Model for Simulating Complex Polydisperse Sprays
Spray application

Dense

Injection nozzle

Primary atomization

Secondary droplet breakup

Droplet-droplet interactions

Evaporation

Dilute
Simulation emphasis

- **Major foci**
  - Atomization of liquid fuel
  - Momentum transfer between phases
  - Droplet-droplet/-turbulence interaction
  - Heat and mass transfer
  - Chemical reactions

- **Major challenges**
  - Small time and size scales
  - Large amount of droplets
  - Varying spray regime

- **Major aspects**
  - Practicable for industrial applications
  - Simulation on a microscopic level is prohibitive
  - Modeling is based on a statistical level of description
Outline

1 Spray modeling
Outline

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2 Method of Moments
   - DQbSMoM
   - Operator splitting

3 Evaporation modeling
   - Equilibrium and non-equilibrium formulation
   - Models under investigation

4 Spray simulation
   - Experimental and numerical configuration
   - Results

5 Summary and outlook
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Spray modeling principles

- Kinetic spray equation of distribution function $f(x, t; u, \phi, T)$

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial x_i} (u_i f) + \frac{\partial}{\partial u_i} (F_i f) + \frac{\partial}{\partial \phi} (R_\phi f) + \frac{\partial}{\partial T} (\theta f) = \Gamma$$

- Physical aspects
  - $\frac{\partial f}{\partial t}$ Transient term
  - $\frac{\partial}{\partial x_i} (u_i f)$ Convective term
  - $\frac{\partial}{\partial u_i} (F_i f)$ Momentum transfer
  - $\frac{\partial}{\partial \phi} (R_\phi f)$ Mass transfer
  - $\frac{\partial}{\partial T} (\theta f)$ Heat transfer
  - $\Gamma$ Droplet-droplet interaction

- Solving approaches

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<th>RANS</th>
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<td>Eulerian moment methods</td>
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Lagrangian and Eulerian methods

- **Stochastic Lagrangian Methods**
  - Robust, accurate and well established
  - RANS/LES simulations with lower parallelization of solver
  - Requiring sufficient amount of parcels to avoid statistical noise
  - High computational cost for highly unsteady simulations with fine mesh
  - Hardly achievable optimal parallelization

  Tendency: LES and highly parallelized simulations

- **Eulerian Moment Methods**
  - Equations of both phases share same structure
  - Straightforward phase coupling
  - Achievable optimal parallelization
  - Under research and majorly used for academic applications
  - Variety of approaches

  Tendency: Growing awareness and interest
Assumptions of MoM

- Approximation of NDF by weighted Dirac-delta functions

\[ f(x, t; u, \phi, T) \approx \sum_{n=1}^{N} w_n \delta(\phi - \phi(x, t)) \delta(u - u_n(x, t)) \delta(T - T_n(x, t)) \] (2)

- Calculation of moments

\[ m_{qlmp\theta}(x, t; u, \phi, T) = \sum_{n=1}^{N} w_n \phi_n^q u_1^l_n u_2^m_n u_3^p_n T_n^\theta \] (3)

- Moments of diameter \((q = d)\)

- \( m_0^d \) amount of droplets
- \( m_1^d \) \( \sim \) mean diameter
- \( m_2^d \) \( \sim \) surface
- \( m_3^d \) \( \sim \) volume/mass
Assumptions of DQbSMoM

- Splitting of \( f(x, t; u, \phi, T) \) into \( k \) sections

\[
f(x, t; u, \phi, T) = \sum_{k=1}^{N_s} f_k(x, t; u, \phi, T)
\]  

(4)

- Utilization of indicator function

\[
f_k(x, t; u, \phi, T) = \begin{cases} 
  f_k(x, t; u, \phi, T) & \text{if } \phi \in [\phi_{k-1}, \phi_k) \\
  0 & \text{otherwise}
\end{cases}
\]

(5)

- Approximation of NDF over each section \( k \)

\[
f_k(x; t, u, \phi, T) \approx \sum_{n=1}^{N} w_{k,n} \delta(d - d_{k,n}) \delta(u - u_{k,n}) \delta(T - T_{k,n})
\]

(6)
Concept of the DQbSMoM

![Graph showing the number density function of droplet diameter.](image)
Concept of the DQbSMoM
Closure strategy

- General approach
  - Insertion of Dirac-delta approximation
  - Application of moment transform
  - Choice of $6 \cdot N$ independent, non-singular moments
  - Linear system is solved using modified standard DQMoM

- Standard DQMoM approach
  - Outcome is a set of 4 Eulerian transport equations
  - Consideration of physical phenomena by source terms on RHS

- DQbSMoM approach
  - Application of operator splitting strategy
  - Separate handling of terms on LHS

- Framework for this method
  - Based on incompressible Finite Volume Method
  - Implicit time discretisation
Operator splitting

Splitting Eq. (1) according to $\frac{\partial f}{\partial t} =$

<table>
<thead>
<tr>
<th>Physical space</th>
<th>Phase space</th>
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<tr>
<td>Multi-fluid method</td>
<td>EMSM and SM</td>
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<tr>
<td>$- \frac{\partial}{\partial x_i} (u_i f) - \frac{\partial}{\partial u_i} (F_i f)$</td>
<td>$- \frac{\partial}{\partial \phi} (R_\phi f) - \frac{\partial}{\partial T} (\theta f)$</td>
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Two-step splitting strategy
- Phase space transport during $\Delta t/2$
- Physical space transport during $\Delta t$
- Phase space transport during $\Delta t/2$

Solving approaches
- EMSM/SM is consistent with evaporation models
- Coalescence is neglected ($\Gamma = 0$)
- Formulation is equivalent to splitting of source terms
Coupling with multi-fluid method

- Basics of coupling approach
  - Inserting volume fraction results in multi-fluid system
  - RHS includes drag term, turbulence diffusion and gravity effects
  - Equivalent to multi-fluid system with $N_s \cdot N$ phases
  - Straightforward coupling, because equations share same structure

- Fundamental assumptions
  - Based on density based averaging strategy
  - Modeling approaches are needed for closure
  - Turbulence of disperse phase is derived by gas phase

- Characteristics of the coupling approach
  - Consideration of $\phi = \nu$
  - Additional transport equations for diameter and temperature abscissae
  - Mono-kinetic assumption
EMS/M in consistency with evaporation

- Features of EMSM/SM
  - Prediction of flux of evaporating droplets at zero size
  - Prediction of moment flux $\psi$ at section boundaries
  - Consideration of $\phi = s$

- Calculation algorithm
  - Approximate NDF and calculate moment vector $M_{\phi_k}$
  - Calculate moment fluxes $\psi$ at each section boundary
  - Modify moment vector and calculate quadrature points
    
    $M_{\phi_k}^{*} = M_{\phi_k} - \psi_{k-1} + \psi_k$
  
  - Shift NDF using general DQMOM approach
    
    $\phi_{k,n}(t + \Delta t) = R_{\phi} \Delta t + \phi_{k,n}(t)$
    $T_{k,n}(t + \Delta t) = \theta \Delta t + T_{k,n}(t)$

- Calculate change of vapor mass fraction
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Equilibrium and non-equilibrium formulation

- **Equilibrium formulation of vapor mole at droplets’ surface**

  \[ X_{s(eq)} = \frac{p_{sat}}{p_g} = \frac{p_{atm}}{p_g} \exp \left( \frac{h_{vap} W_d}{R} \left( \frac{1}{T_{boil}} - \frac{1}{T_d} \right) \right) \]  
  \( (7) \)

- **Non-equilibrium formulation**

  \[ X_{s(neq)} = X_{s(eq)} - \left( \frac{2 L_k}{d} \right) \beta \]  
  \( (8) \)

- **Advantages of non-equilibrium evaporation models**
  - High temperature difference
  - Minor droplet diameter
  - High relative velocity

\[ L_k = \frac{\mu_g \sqrt{2 \pi T_d R/W_d}}{\alpha_e Sc_g p_g} \]  
\[ \beta = - \left( \frac{3 Pr_g \tau_d}{2} \right) \frac{\dot{m}_d}{m_d} \]
Models under investigation

- Equilibrium model by Abramzon and Sirignano (1989)
- Non-equilibrium model by Langmuir and Knudsen (1978)
- Evaporation rate and transient droplet temperature

\[
\frac{dm_d}{dt} = - \frac{Sh}{3 \text{ } Sc_g} \left( \frac{m_d}{\tau_d} \right) H_M \tag{9}
\]

\[
\frac{dT_d}{dt} = \frac{f_d Nu}{3 \text{ } Pr_g} \left( \frac{c_{p,g}}{c_{p,v}} \right) \left( T_g - T_d \right) + \left( \frac{h_{\text{vap}}}{c_{p,d}} \right) \frac{\dot{m}_d}{m_d} \tag{10}
\]

- Varying formulation for $H_M$ and $f_d$
- Sherwood and Nusselt number

\[
Sh = 2 + 0.522 \text{ } Re_d^{\frac{1}{2}} \text{ } Sc_g^{\frac{1}{3}} \quad Nu = 2 + 0.522 \text{ } Re_d^{\frac{1}{2}} \text{ } Pr_g^{\frac{1}{3}} \tag{11}
\]

- Reference values $T_{\text{ref}}$ and $Y_{\text{ref}}$ according $^{1/3}$-rule
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Experimental configuration

- Non-reacting acetone spray
- Jet surrounded by a pilot and a coflow
- \( T_g = T_d = 300 \text{ K}, \ p_g = 0.1 \text{ MPa} \)
- Ultrasonic nebulizer for spray
- Usage of Laser Doppler Velocimetry and Phase Doppler Particle Anemometry
- 7 measurement positions above the nozzle exit \((x/D = 0.3; \ldots; 30)\)

<table>
<thead>
<tr>
<th></th>
<th>( u_{jet} )</th>
<th>( u_{pilot}, u_{coflow} )</th>
<th>( \dot{m}_{jet} )</th>
<th>( \dot{m}_d )</th>
<th>( \dot{m}_{d(l)} )</th>
<th>( \dot{m}_{d(g)} )</th>
<th>( Re )</th>
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<td>SP1</td>
<td>24.0</td>
<td>4.5</td>
<td>150.0</td>
<td>75.0</td>
<td>22.1</td>
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<tr>
<td>SP6</td>
<td>36.0</td>
<td>4.5</td>
<td>225.0</td>
<td>45.0</td>
<td>28.5</td>
<td>16.5</td>
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Numerical configuration

- Turbulence of gas phase is described with modified $k-\varepsilon$ model
- Approx. lognormal size distribution
- *slip wall* condition for cylinders’ surface
- Inlet is located at $x/D = 0.3$
- Smallest cells have a length of 0.5 mm
- 5 subiterations for evaporation model
- Polynomials for thermodynamic variables

<table>
<thead>
<tr>
<th>Radius</th>
<th>Height</th>
<th>$\Delta t$</th>
<th>CV number</th>
<th>Points</th>
<th>Sections $k$</th>
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<tr>
<td>mm</td>
<td>mm</td>
<td>s</td>
<td>$\sim 350,000$</td>
<td>6</td>
<td>3</td>
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<td>SP1/SP6</td>
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<td>$1.5 \times 10^{-5}$</td>
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Results

Droplet mean surface diameter

Droplet Sauter mean diameter
Results

Droplet concentration

Droplet flux

Volume flux \([\text{m}^3/(\text{m}^2 \text{s})]\)
Results

Mean axial velocity

Mean radial velocity

SP1 SP6

x/D = 30

x/D = 25

x/D = 20

x/D = 15

x/D = 10

SP1 SP6

x/D = 30

x/D = 25

x/D = 20

x/D = 15

x/D = 10

SP1 SP6
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Summary and outlook

- Modeling approach
  - Modeling multiphase flows
  - Method of Moments
  - Operator splitting approach
  - Evaporation modeling

- Results for SP1 and SP6
  - Experimental and numerical configuration
  - Results for equilibrium and non-equilibrium model

- Coupling to a combustion model
  - Single droplet combustion experiments
  - Spray combustion experiments

- Improvements of turbulence modeling

...
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