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

Advanced Hybrid Model for Simulating Complex Polydisperse Sprays

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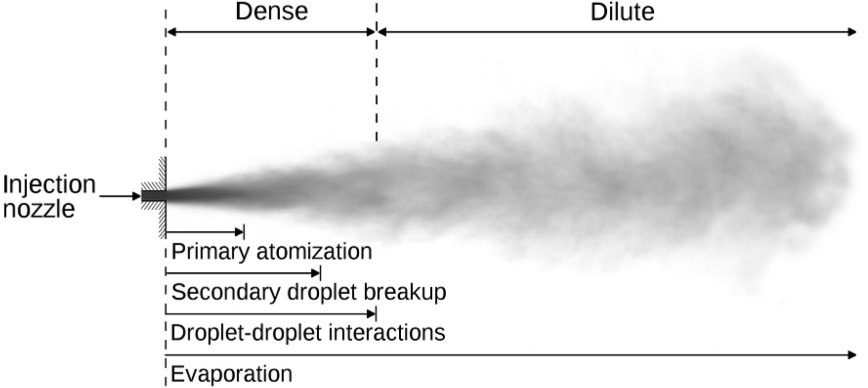
Spray application



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

1. Spray modeling
2. Method of Moments
    - DQbSMoM
    - Operator splitting

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

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   - Experimental and numerical configuration
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Spray modeling principles

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

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial x_i}(u_i f) + \frac{\partial}{\partial u_i}(F_i f) + \frac{\partial}{\partial \phi}\left(R_\phi f\right) + \frac{\partial}{\partial T}(\theta f) = \Gamma \tag{1}$$

- 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	$\frac{\partial}{\partial \phi}\left(R_\phi f\right)$	Mass transfer
$\frac{\partial}{\partial T}(\theta f)$	Heat transfer	Γ	Droplet-droplet interaction

- Solving approaches

DNS	LES	RANS
Stochastic Lagrangian methods		Eulerian moment methods
Microscopic models	Mesoscopic models	Macroscopic models

Lagrangian and Eulerian methods

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- 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

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Assumptions of MoM

- Approximation of NDF by weighted Dirac-delta functions

$$f(\mathbf{x}, t; \mathbf{u}, \phi, T) \approx \sum_{n=1}^{N} w_n \, \delta(\phi - \phi(\mathbf{x}, t)) \, \delta(\mathbf{u} - \mathbf{u}_n(\mathbf{x}, t)) \, \delta(T - T_n(\mathbf{x}, t)) \qquad (2)$$

- Calculation of moments

$$m_{qlmp\theta}(\mathbf{x}, t; \mathbf{u}, \phi, T) = \sum_{n=1}^{N} w_n \phi_n^q u_{1,n}^l u_{2,n}^m u_{3,n}^p T_n^\theta \qquad (3)$$

- Moments of diameter ($q = d$)

m_d^0	amount of droplets	m_d^1	$\sim$ mean diameter
m_d^2	$\sim$ surface	m_d^3	$\sim$ volume/mass

Assumptions of DQbSMoM

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

$$f(\mathbf{x}, t; \mathbf{u}, \phi, T) = \sum_{k=1}^{N_s} f_k(\mathbf{x}, t; \mathbf{u}, \phi, T) \tag{4}$$

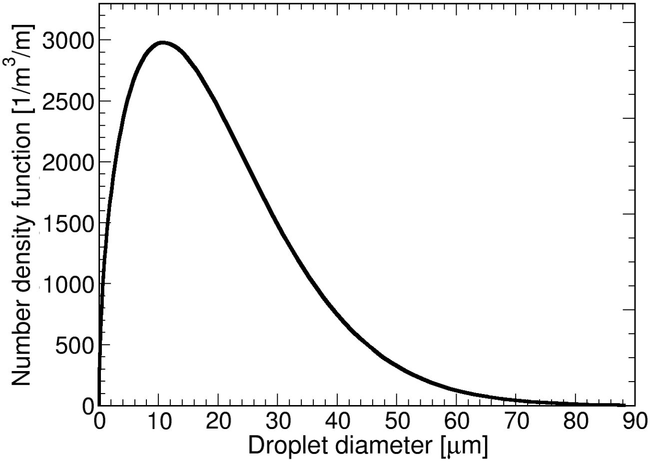
- Utilization of indicator function

$$f_k(\mathbf{x}, t; \mathbf{u}, \phi, T) = \begin{cases} f_k(\mathbf{x}, t; \mathbf{u}, \phi, T) & \text{, if } \phi \in [\phi_{k-1}, \phi_k) \\ 0 & \text{, otherwise} \end{cases} \tag{5}$$

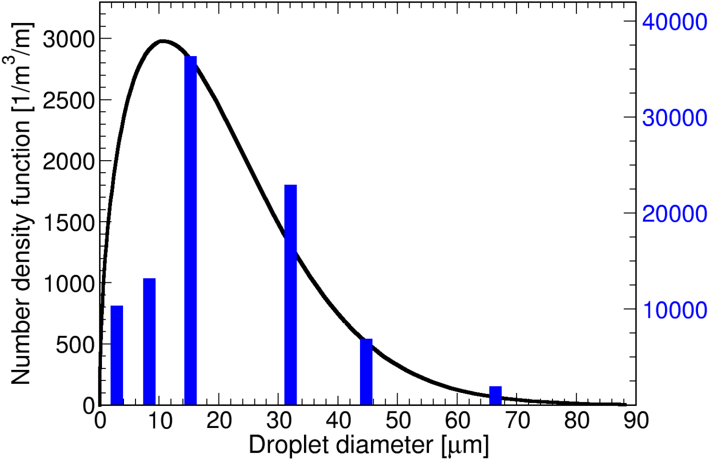
- Approximation of NDF over each section k

$$f_k(\mathbf{x}; t, \mathbf{u}, \phi, T) \approx \sum_{n=1}^{N} w_{k,n}\, \delta\left(d - d_{k,n}\right) \delta\left(\mathbf{u} - \mathbf{u}_{k,n}\right) \delta\left(T - T_{k,n}\right) \tag{6}$$

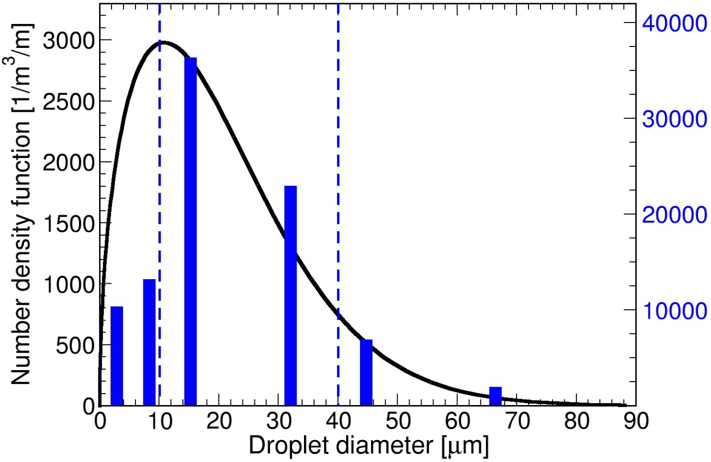
Concept of the DQbSMoM



Concept of the DQbSMoM



Concept of the DQbSMoM



Closure strategy

- General approach
  - Insertion of Dirac-delta approximation
  - Application of moment transform
  - Choice of $6 \cdot N$ indepent, 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 $\frac{\partial f}{\partial t} =$

Physical space	Phase space	
Multi-fluid method	EMSM and SM	Coalescence algorithm
$-\frac{\partial}{\partial x_i}(u_i f) - \frac{\partial}{\partial u_i}(F_i f)$	$-\frac{\partial}{\partial \phi}\left(R_\phi f\right) - \frac{\partial}{\partial T}(\theta f)$	Γ

- Two-step splitting strategy
  - Phase space transport during $^{\Delta t}/_2$
  - Physical space transport during Δt
  - 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 $\phi = \upsilon$
  - Additional transport equations for diameter and temperature abscissae
  - Mono-kinetic assumption

EMSM/SM in consistency with evaporation

- Features of EMSM/SM
  - Prediction of flux of evaporating droplets at zero size
  - Prediction of moment flux ψ at section boundaries
  - Consideration of $\phi = s$
- Calculation algorithm
  - Approximate NDF and calculate moment vector M_{ϕ_k}
  - Calculate moment fluxes ψ 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

Outline

Equilibrium and non-equilibrium formulation

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- Equilibrium formulation of vapor mole at droplets' surface

$$X_{\mathrm{s(eq)}} = \frac{p_{\mathrm{sat}}}{p_{\mathrm{g}}} = \frac{p_{\mathrm{atm}}}{p_{\mathrm{g}}} \exp\left(\frac{h_{\mathrm{vap}} W_{\mathrm{d}}}{R}\left(\frac{1}{T_{\mathrm{boil}}} - \frac{1}{T_{\mathrm{d}}}\right)\right) \tag{7}$$

- Non-equilibrium formulation

$$X_{\mathrm{s(neq)}} = X_{\mathrm{s(eq)}} - \left(\frac{2L_{\mathrm{k}}}{d}\right)\beta \tag{8}$$

$$L_{\mathrm{k}} = \frac{\mu_{\mathrm{g}}\sqrt{2\pi T_{\mathrm{d}}\, {}^{R}\!/\!{}_{W_{\mathrm{d}}}}}{\alpha_e\, Sc_{\mathrm{g}}\, p_{\mathrm{g}}} \qquad \beta = -\left(\frac{3\, Pr_{\mathrm{g}}\, \tau_{\mathrm{d}}}{2}\right)\frac{\dot{m}_{\mathrm{d}}}{m_{\mathrm{d}}}$$

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

Models under investigation

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

$$\frac{\mathrm{d}m_\mathrm{d}}{\mathrm{d}t} = -\frac{Sh}{3\,Sc_\mathrm{g}} \left(\frac{m_\mathrm{d}}{\tau_\mathrm{d}}\right) H_\mathrm{M} \tag{9}$$

$$\frac{\mathrm{d}T_\mathrm{d}}{\mathrm{d}t} = \frac{f_\mathrm{d}\,Nu}{3\,Pr_\mathrm{g}} \left(\frac{c_\mathrm{p,g}/c_\mathrm{p,v}}{\tau_\mathrm{d}}\right) \left(T_\mathrm{g} - T_\mathrm{d}\right) + \left(\frac{h_\mathrm{vap}}{c_\mathrm{p,d}}\right) \frac{\dot{m}_\mathrm{d}}{m_\mathrm{d}} \tag{10}$$

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

$$Sh = 2 + 0.522\,Re_\mathrm{d}^{\frac{1}{2}}\,Sc_\mathrm{g}^{\frac{1}{3}} \qquad Nu = 2 + 0.522\,Re_\mathrm{d}^{\frac{1}{2}}\,Pr_\mathrm{g}^{\frac{1}{3}} \tag{11}$$

- Reference values T_ref and Y_ref according $^1/_3$*-rule*

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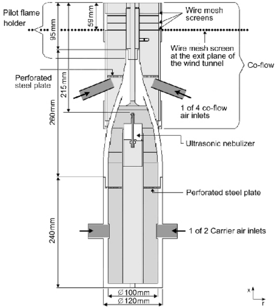
Experimental configuration

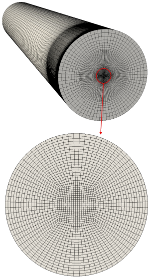
- Non-reacting acetone spray
- Jet surrounded by a pilot and a coflow
- $T_g = T_d = 300\,\mathrm{K}$, $p_g = 0.1\,\mathrm{MPa}$
- Ultrasonic nebulizer for spray
- *Usage of Laser Doppler Velocimetry* and *Phase Doppler Particle Anemometry*
- 7 measurement positions above the nozzle exit ($x/D = 0.3;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



	u_{jet}	$u_{\mathrm{pilot}}, u_{\mathrm{coflow}}$	$\dot{m}_{\mathrm{jet}}$	$\dot{m}_{\mathrm{d}}$	$\dot{m}_{\mathrm{d}(l)}$	$\dot{m}_{\mathrm{d}(g)}$	Re
	m/s		g/min		g/min at $x/D = 0.3$		–
SP1	24.0	4.5	150.0	75.0	22.1	52.9	24,288
SP6	36.0	4.5	225.0	45.0	28.5	16.5	27,937

Numerical configuration

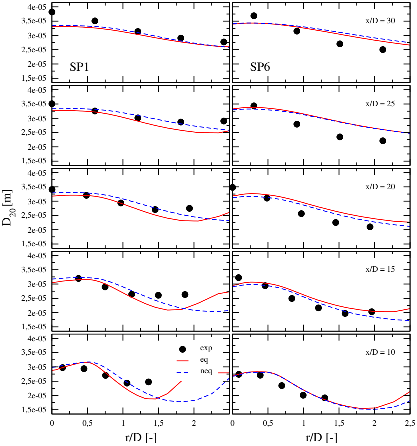
- Turbulence of gas phase is described with modified k-ε model
- Approx. lognormal size distribution
- *slip wall* condition for cylinders' surface
- Inlet is located at $x/D = 0.3$
- Smallest cells have a length of 0.5 mm
- 5 subiterations for evaporation model
- Polynomials for thermodynamic variables



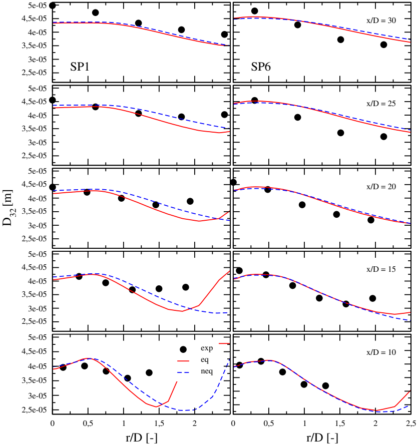
	Radius	Hight	Δt	CV number	Points	Sections k
	mm	mm	s	–	–	–
SP1/SP6	50	500	1.5×10^{-5}	$\sim$ 350,000	6	3

Results

Droplet mean surface diameter



Droplet Sauter mean diameter



Results

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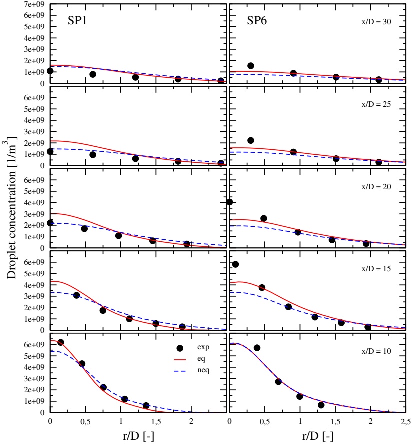
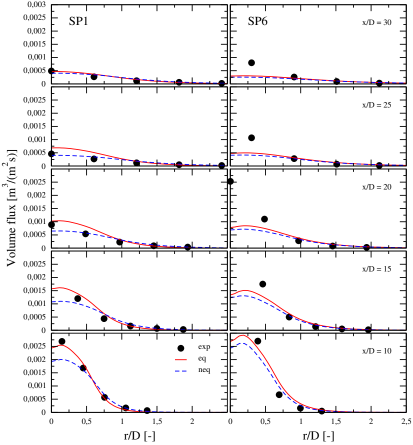
Droplet concentration

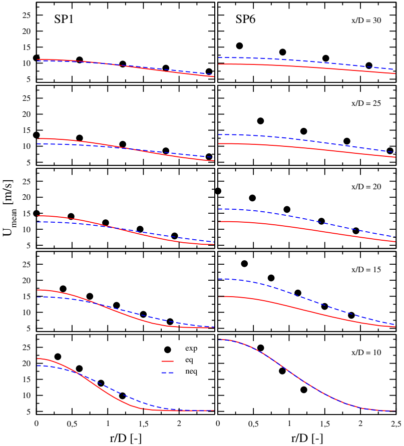


Droplet flux

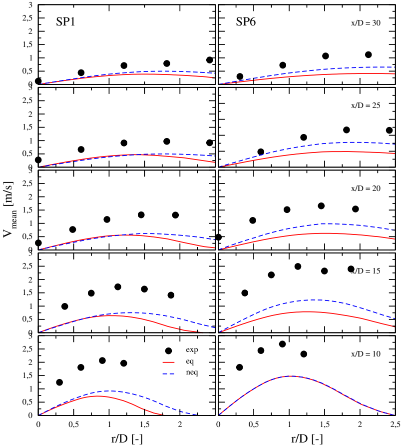


Results

Mean axial velocity



Mean radial velocity



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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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