Weierstrass Institute for
Applied Analysis and Stochastics

# On numerical methods for the simulation of two-phase flows with population balance systems

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in collaboration with:
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# Content

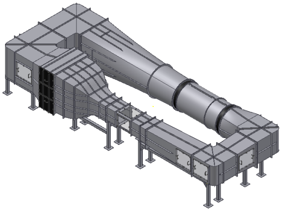
## Motivation

- Simulation of two phase wind tunnel experiments
- Development of robust, accurate, and efficient numerical schemes for simulations of population balance systems
- Population balance system describe evolutions of the droplet size distribution, not the behavior of individual droplets
- Modeling point of view: coupled systems of
  - Navier–Stokes equations (turbulent air flow, 3D)
  - Droplet size distribution equation (droplets, integro partial differential equation, 4D)

$\Longrightarrow$ Equations are defined in domains with different dimensions

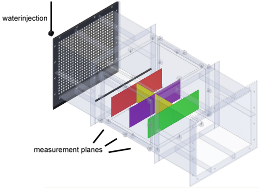
# Motivation

- Simulation of wind tunnel experiments, comparison of numerical and experimental data (Bordás, Thévenin)



Experiment

- Horizontal wind tunnel
- Two phase flow
  - Turbulent air flow
  - Water droplet distribution
- Droplet motion in turbulent flows
- Aggregation of droplets




Experimental Data

- Available on three planes perpendicular to the flow direction
- Used as boundary condition for simulation (inlet) and for evaluation of the results (outlet)
- Important data: flow velocity, droplet size distribution, droplet velocity

## Mathematical Model

### Turbulent flow

- Incompressible Navier–Stokes equations

$$\begin{aligned} \partial_t \mathbf{u} - 2\nabla \cdot (\mathrm{Re}^{-1}\mathbb{D}(\mathbf{u})) + (\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p &= \mathbf{0} \quad \text{in } (0,T]\times\Omega \\ \nabla\cdot\mathbf{u} &= 0 \quad \text{in } [0,T]\times\Omega \end{aligned}$$

- Flow domain and boundary conditions given by experimental data
- Grid incorporates points of measurements as nodes
- Turbulence modeling
  - Variational multiscale finite element VMS method, John, Kaya (2005)
  - Variational multiscale finite element VMS method with adaptive large scale space, John, Kindl (2010)

## Mathematical Model

- 4D droplet size distribution equation

$$
\begin{aligned}
& f_t + \mathbf{u}_{\text{drop}} \cdot \nabla_{\mathbf{x}} f + \left(\frac{a}{d} f\right)_d \\
& = \frac{d^2}{2} \int_{d_{\min}}^{d} \frac{\kappa_{\text{agg}}\left((d^3 - d'^3)^{\frac{1}{3}}, d'\right)}{(d^3 - d'^3)^{\frac{2}{3}}} f\left(\cdot, (d^3 - d'^3)^{\frac{1}{3}}\right) f(\cdot, d')\, dd' \\
& - f(\cdot, d) \int_{d_{\min}}^{d_{\max}} \kappa_{\text{agg}}(d, d') f(\cdot, d')\, dd' \quad \text{in } (0, T] \times \Omega \times [d_{\min}, d_{\max}]
\end{aligned}
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- In the model are included
  - Motion in turbulent flow $\Longrightarrow$ transport-dominated equation
  - Growth in supersaturated air
  - Aggregation

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- Droplet-size distribution
- Droplet velocity (Navier–Stokes Equation-(space-time averaged slip velocity))

  $\Rightarrow$ coupling to the Navier–Stokes equation
- Growth constant
- Droplet diameter
- Aggregation kernel

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## Aggregation

- Convolution integral
  - Simple two-loop scheme very slow
  - Integrand nearly singular: if standard quadrature rules are used $\Longrightarrow$ poor accuracy $\Longrightarrow$ considerable loss of mass
- Current approach: evaluation of the aggregation term bases on a preprocessing step

$$
\begin{aligned}
& f(d[j]) \int_{d_{\min}}^{d_{\max}} \kappa_{\text{agg}}(d[j], d') f(d')\, dd' \\
&= f(d[j]) \sum_{i=1}^{N_a-1} \int_{d[i]}^{d[i+1]} \kappa_{\text{agg}}(d[j], d') f(d')\, dd' \\
&\approx f(d[j]) \sum_{i=1}^{N_a-1} \frac{f(d[i+1]) + f(d[i])}{2} \underbrace{\int_{d[i]}^{d[i+1]} \kappa_{\text{agg}}(d[j], d')\, dd'}_{\text{preprocessed integrals}}
\end{aligned}
$$

- Remaining integrals depend only on the kernel and the grid for the internal coordinate, can be computed in preprocessing step
- More efficient and accurate than simple approach
- But still some loss of mass

# Aggregation

- Work in progress
  - More efficient scheme from Hackbusch (2007)
  - Implement scheme on basis of mass instead of diameters
    $\Rightarrow$ Singularity smaller
    $\Rightarrow$ Smaller numerical errors expected

- Aggregation kernel
  - Model consists of two parts: Brownian motion and shear induced motion

$$\kappa_{\mathrm{agg}} = C_{\mathrm{brown}} \frac{2k_B T}{3\mu}(d+d')\left(\frac{1}{d}+\frac{1}{d'}\right) + C_{\mathrm{shear}} \sqrt{2\nabla \mathbf{u} : \nabla \mathbf{u}}\,(d+d')^3$$

  - $C_{\mathrm{brown}}$ and $C_{\mathrm{shear}}$: unknown parameters
  - Parameter identification by comparison with experimental data

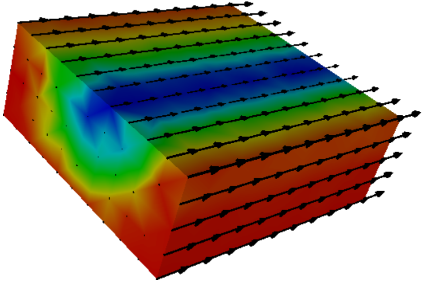
# Numerical Methods for Transport-Dominated Equations

- Efficient and accurate numerical method for the 4D transport equation necessary; see John, Roland (2010)
- Available methods
  - Forward/backward Euler + finite difference upwind (fast, rather inaccurate)
  - Crank–Nicolson + linear FEM–FCT; Kuzmin (2009) (rather slow, accurate)
  - Finite Difference ENO schemes with explicit TVD Runge–Kutta
- Work in progress
  - FEM–FCT with Group FEM, Fletcher (1973)

## Simulation of the Experiments – The Flow Field

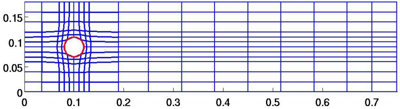
- $\Omega$ : 51 x 46 x 19 nodes, hexahedral grid
- $\Delta t = 0.001$
- $Q_2/P_1^{\text{disc}}$ finite element method
- Crank–Nicolson scheme
- Simulations with the code MooNMD

Snap shot of the computed velocity field

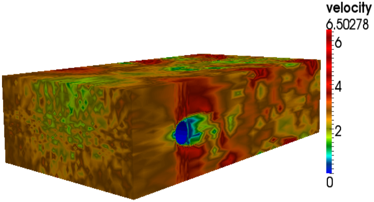


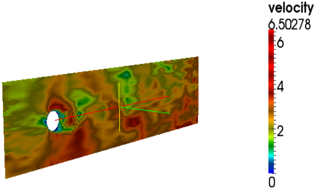
# The Flow Field - - Flow around a cylinder

- coarse grid for the multiscale solver



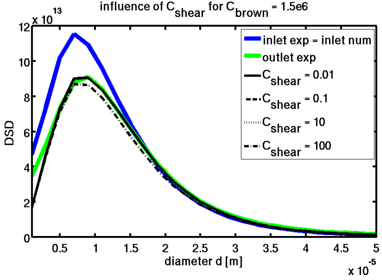

- d.o.f.: 1 000 000, hexahedral grid
- time step: $\Delta t = 5e-3$



## Simulation of the Experiments – Calibration of Parameters

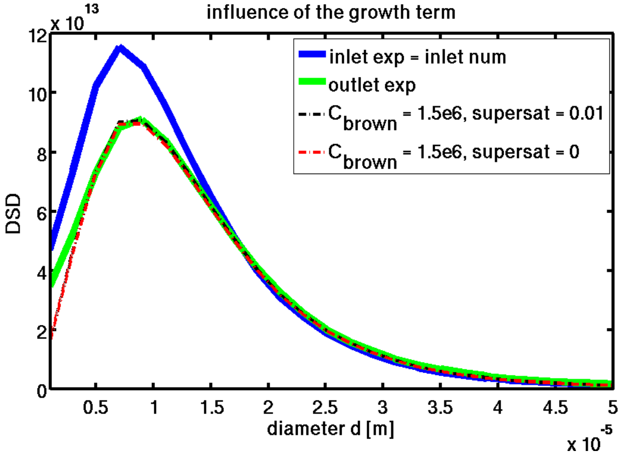
- Calibration of the parameters $C_{\mathrm{brown}}$ and $C_{\mathrm{shear}}$ of the aggregation kernel
- Used method for calibration: forward Euler scheme




- Good agreement for suitable chosen parameters $C_{\mathrm{brown}} = 1.5e6$ and $C_{\mathrm{shear}} \in [0.01, 1]$

## Simulation of the Experiments – Aggregation vs. Growth

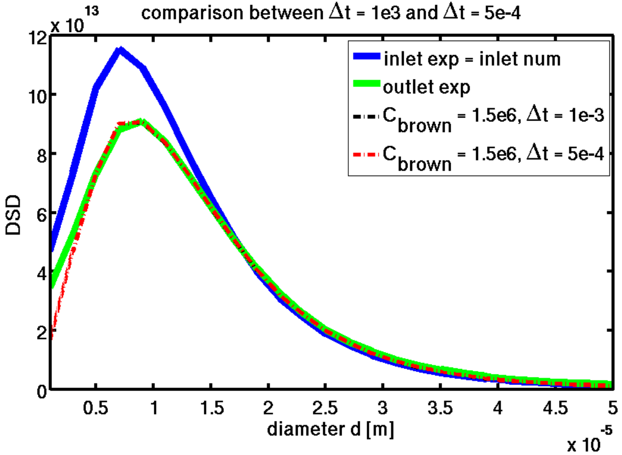
- Simulations without growth (supersaturation = 0)




- Dominant aggregation corresponds to physics of the problem

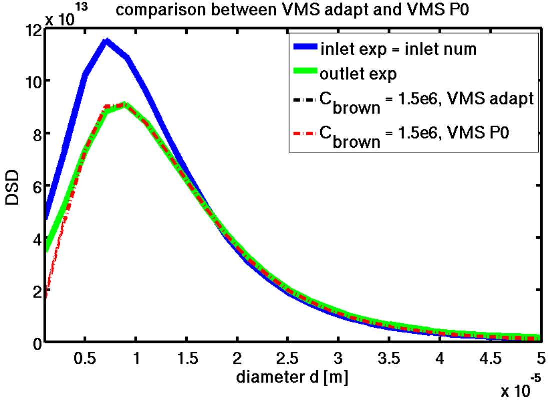
# Simulation of the Experiments – Robustness w.r.t. Methods

- Different length of the time step
  - $\Delta t = 10^{-3}$ vs. $\Delta t = 5 \cdot 10^{-4}$



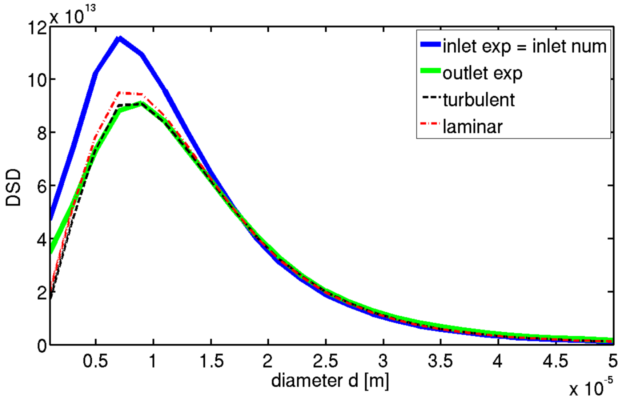
# Simulation of the Experiments – Robustness w.r.t. Methods

- Different turbulence models
  - Finite element VMS method with projection space $P_0$
  - Finite element VMS method with adaptively chosen projection space



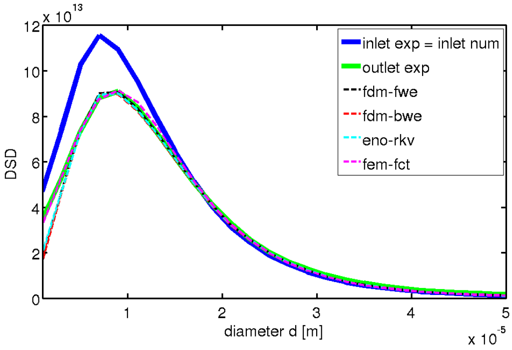
# Simulation of the Experiments – Robustness w.r.t. Methods

- Laminar flow – extension of experimental mean velocity at inlet to the whole domain
- Goal: check the influence of the turbulence on the psd



## Simulation of the Experiments – Robustness w.r.t. Methods

- Different methods for the population balance equation




| method | computing time per time step |
|---|---|
| forward Euler + finite difference upwinding | 178s $\approx$ 3min. |
| backward Euler + finite difference upwinding | 329s $\approx$ 6min |
| explicit Runge–Kutta + Eno | 195s $\approx$ 3.25min |
| Crank–Nicolson + FEMFCT | 857s $\approx$ 14.5min |

## Conclusions and Outlook

- Conclusions
  - Calibration of parameters in aggregation kernel to match experimental data could be performed
  - Experiments could be simulated quite accurately
  - Results robust with respect to numerical methods
  - Flow field around cylinder calculated
- Outlook
  - Next experiment: flow around a cylinder: Droplet Distribution has to be calculated
  - Alternative methods for transport equation
    - FEM–FCT with Group FEM, Fletcher (1973)
  - Aggregation term
    - Formulation in terms of mass instead of diameter
    - Method by Hackbusch

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