Modelling Two-Phase Flows by Single Phase RANS and Population Dynamics

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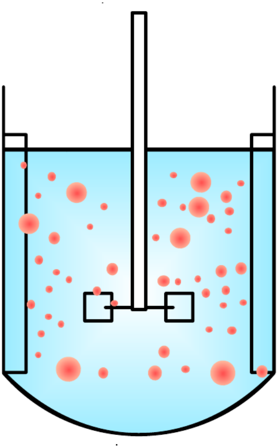
- Stirring of two fluids
- Reynoldsnumber $Re \sim 30,000$
- In industrial applications:
  - continuous phase $\sim 90\%$
  - dispersed phase $\sim 10\%$
- Imagine droplets of oil swimming in water



Numerical simulation of the stirring process

Physical model that is

- Two phases
- Phase interactions
- Inhomogeneous turbulent flow field

simplified for simulations

- One phase (mixture)
- Distribution of dispersion is determined by the flow of the mixture
- Low-fidelity turbulence modelling

\+ Numerical errors

Justification for the reduced model:

1. Volume fraction $\phi \sim 10\%$ of the dispersed phase is small
2. Physical properties (density, viscosity) of the phases are similar

And thus one assumes that

- The mixture behaves like a single fluid
- Droplets simply move with the fluid
- No phase interaction

Manifold motivations of analysing the model:

- Quantify the validity regions
- Balance the numerical error and the modelling error
- Capture tendencies like overestimation
- Improve the model

Outline of the talk

Start with a microscopic for every droplet and do

1. Averaging
2. Summation of the phases
3. Modelling of interactions and turbulence
4. Modelling of the dispersed phase

to come up with a global macroscopic model for the mixture

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Averaging of flow variables $f(t,x)$:

- e.g. time averaging:

$$\langle \psi \rangle (t,x) := \frac{1}{\hat{t}} \int_{t-\hat{t}}^{t} \psi(\tau, x) \mathrm{d}\tau$$

with a suitable averaging period $\hat{t}$

- Properties

$$\langle \psi + \varphi \rangle = \langle \psi \rangle + \langle \varphi \rangle, \qquad \langle \langle \psi \rangle \varphi \rangle = \langle \psi \rangle \langle \varphi \rangle,$$

$$\langle \frac{\partial \psi}{\partial t} \rangle = \frac{\partial \langle \psi \rangle}{\partial t}, \qquad \langle \frac{\partial \psi}{\partial x_i} \rangle = \frac{\partial \langle \psi \rangle}{\partial x_i}$$

- But in general

$$\langle \psi \varphi \rangle \neq \langle \psi \rangle \langle \varphi \rangle.$$

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Decompositions of flow variables $\psi(t,x)$

- into averaged (mean) and fluctuating part:

$$\psi(t,x) = \langle\psi\rangle(t,x) + \psi'(t,x)$$

- with

$$\langle\langle\psi\rangle\rangle = \langle\psi\rangle \quad \text{and} \quad \langle\psi'\rangle = 0$$

- for the velocity v and the stresses T

$$v = \langle v\rangle + v' \quad \text{and} \quad T = \langle T\rangle + T'$$

but not for the densities $\rho = \langle\rho\rangle$.

Phase-indicator funktion

$$\chi_d(t,x) = \begin{cases} 1 & \text{if } x \text{ is in the dispersed phase at time } t \\ 0 & \text{otherwise} \end{cases} .$$

Treating χ_d as a generalized function one can find

$$\frac{\partial \chi_d}{\partial t} + v \cdot \nabla \chi_d = 0.$$

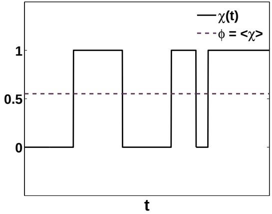
and justify the notation

$$\nabla \chi_d = n_d \frac{\partial \chi_d}{\partial n}.$$

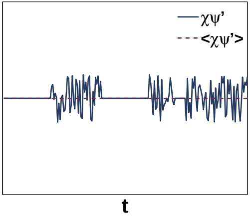
The term $\frac{\partial \chi_d}{\partial n}$ acts like a δ-function by picking out the boundaries of the dispersed phase.

Putting all concepts together one can reason

- $\langle \chi_d \rangle = \phi$
  (Dispersed phase fraction)



- $\langle \chi_d \psi \rangle = \phi \langle \psi \rangle$ and $\langle \chi_d \psi' \rangle = 0$



- $\langle \psi' \nabla \chi_d \rangle = 0$
  (Boundary average)

which will be of major importance in the modelling.

For phase α in a multiphase flow one has

$$\frac{\partial \rho_\alpha}{\partial t} + \nabla \cdot \rho_\alpha v = 0$$
$$\frac{\partial \rho_\alpha v}{\partial t} + \nabla \cdot \rho_\alpha v v - \nabla \cdot T_\alpha - \rho_\alpha f = 0$$

in the interior, with the tensor of stresses

$$T_\alpha = -pI + \mu_\alpha[\nabla v + (\nabla v)^T]$$

and the interfaces the jump conditions

$$[\![\rho_\alpha(v - v_s) \cdot n]\!] = 0$$
$$[\![\rho_\alpha v(v - v_s) \cdot n - T_\alpha \cdot n]\!] = \sigma \kappa n$$

ρ_α ... density
μ_α ... viscosity
f ... volume force
v_s ... interface v
n ... normal vector
κ ... curvature
σ ... interfacial tension

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Exemplarily for the dispersed phase for the continuum equation

$$\frac{\partial \rho_d}{\partial t} + \nabla \cdot \rho_d v = 0$$

Multiply by χ_d and decompose $v = \langle v \rangle + v'$:

$$\chi_d \frac{\partial \rho_d}{\partial t} + \chi_d \nabla \cdot \rho_d \langle v \rangle + \chi_d \nabla \cdot \rho_d v' = 0$$

Rearrange by product rule, e.g.

$$\chi_d \frac{\partial \rho_d}{\partial t} = \frac{\partial \chi_d \rho_d}{\partial t} - \rho_d \frac{\partial \chi_d}{\partial t} = \frac{\partial \chi_d \rho_d}{\partial t} + \rho_d v_s \cdot \nabla \chi_d$$

Apply the averaging to the whole equation to cancel out fluctuating terms like

$$\langle \chi_d \nabla \cdot \rho_d v' \rangle = \phi \nabla \cdot \rho_d \langle v' \rangle = 0$$

- Result: The averaged continuum equation for the dispersed phase

$$\frac{\partial \phi\rho_d}{\partial t} + \nabla \cdot \phi\rho_d \langle v \rangle = \langle [\rho_d(\langle v \rangle - v_s)]_d \cdot \nabla \chi_d \rangle.$$

- Similar actions for the momentum equation deliver:

$$\frac{\partial \phi\rho_d \langle v \rangle}{\partial t} + \nabla \cdot \phi\rho_d \langle v \rangle \langle v \rangle - \nabla \cdot \phi T_d^* - \phi\rho_d f = \\ = \langle [\rho_d \langle v \rangle (\langle v \rangle - v_s) - T_d^*] \cdot \nabla \chi_d \rangle.$$

with the tensor of turbulent stresses $T_d^* := \langle T \rangle_d - \rho_d \langle v' v' \rangle$

- Replace the subscript d by c and ϕ by $1 - \phi$ to get these equations for the continuous phase as well.

The right hand sides contain the averaged phase interface conditions

- For the continuum:

$$\left\langle [\rho_d(\langle v \rangle - v_s)]_d \cdot \nabla \chi_d \right\rangle = \left\langle [\![\rho_\alpha(\langle v \rangle - v_s) \cdot n]\!] \right\rangle = 0$$

- For the momentum:

$$\begin{aligned} &\left\langle [\rho_d \langle v \rangle (\langle v \rangle - v_s) - T_d^*] \cdot \nabla \chi_d \right\rangle = \\ &\quad [\![\rho_\alpha \langle v \rangle (\langle v \rangle - v_s) \cdot n - T_\alpha^* \cdot n]\!] = \sigma^* \kappa n := M_d^* \end{aligned}$$

  where σ^* is the turbulent interfacial tension.

- And for the equations corresponding to the continuous phase

Having introduced the symbols for the differences

$$\delta_\rho = \rho_c - \rho_d \quad \text{and} \quad \delta_T^* = \langle T_c \rangle - \langle T_d \rangle - \delta_\rho \langle v' v' \rangle$$

one can sum up the phase equations to get the equations of motion for the mixture

$$\frac{\partial \rho_c}{\partial t} + \nabla \rho_c \langle v \rangle = \frac{\partial \phi \delta_\rho}{\partial t} + \nabla \phi \delta_\rho \langle v \rangle$$

$$\frac{\partial \rho_c \langle v \rangle}{\partial t} + \nabla \rho_c \langle v \rangle \langle v \rangle - \nabla T_c^* - \rho_c f = \frac{\partial \phi \delta_\rho \langle v \rangle}{\partial t} + \nabla \phi \delta_\rho \langle v \rangle \langle v \rangle - $$

$$- \nabla \phi \delta_{T^*} - \phi \delta_\rho f + M_d^* + M_c^*.$$

- T^* and M^* have to be modelled
- Then a population balance equation $P(\phi, \langle v \rangle, T^*) = 0$ closes the system:

$$\frac{\partial \rho_c}{\partial t} + \nabla \rho_c \langle v \rangle = \frac{\partial \phi \delta_\rho}{\partial t} + \nabla \phi \delta_\rho \langle v \rangle$$

$$\frac{\partial \rho_c \langle v \rangle}{\partial t} + \nabla \rho_c \langle v \rangle \langle v \rangle - \nabla T_c^* - \rho_c f = \frac{\partial \phi \delta_\rho \langle v \rangle}{\partial t} + \nabla \phi \delta_\rho \langle v \rangle \langle v \rangle - \\ - \nabla \phi \delta_{T^*} - \phi \delta_\rho f + M_d^* + M_c^*$$

$$0 = P(\phi, \langle v \rangle, T^*)$$

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For the simulation we assumed that ϕ is small and the phases are similar, e.g.

$$\delta_\rho \to 0, \quad \delta_T^* \to 0 \quad \text{and} \quad M_c^* \approx -M_d^*$$

which intuitively justifies the model that neglects the right hand side:

$$\frac{\partial \rho_c}{\partial t} + \nabla \rho_c \langle v \rangle = \frac{\partial \phi \delta_\rho}{\partial t} + \nabla \phi \delta_\rho \langle v \rangle$$

$$\frac{\partial \rho_c \langle v \rangle}{\partial t} + \nabla \rho_c \langle v \rangle \langle v \rangle - \nabla T_c^* - \rho_c f = \frac{\partial \phi \delta_\rho \langle v \rangle}{\partial t} + \nabla \phi \delta_\rho \langle v \rangle \langle v \rangle - \\ - \nabla \phi \delta_{T^*} - \phi \delta_\rho f + M_d^* + M_c^*$$

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$$\begin{aligned} \frac{\partial \rho_c}{\partial t} + \nabla \rho_c \langle v \rangle &= 0 \\ \frac{\partial \rho_c \langle v \rangle}{\partial t} + \nabla \rho_c \langle v \rangle \langle v \rangle - \nabla T_c^* - \rho_c f &= 0 \\ &\quad - 0 \\ 0 &= 0 \end{aligned}$$

Conclusion

- A framework that combines the macroscopic and the turbulence modelling in one equation system has been derived
- The modelling error can be expressed explicitly

And outlook

- Analysis of the asymptotic behavior $\delta_\rho \rightarrow 0$
- Inclusion of numerical errors
- Design of observers for a robust extraction of values of interest from the computed flow variables

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Thanks to Volker Mehrmann for the support and

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For suggestions and questions please contact me

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