

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

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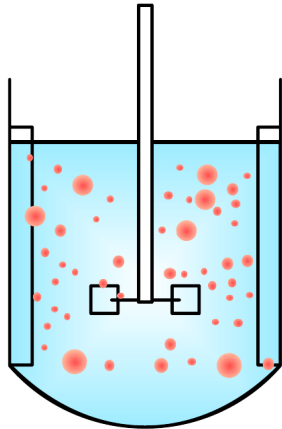
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- Stirring of two fluids
- Reynoldsnumber  $Re \sim 30,000$
- In industrial applications:
  - continuous phase  $\sim 90\%$
  - dispersed phase  $\sim 10\%$
- Imagine droplets of oil swimming in water



## 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

Averaging of flow variables  $f(t, \mathbf{x})$ :

- e.g. time averaging:

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

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

- Properties

$$\begin{aligned} \langle \psi + \varphi \rangle &= \langle \psi \rangle + \langle \varphi \rangle, & \langle \langle \psi \rangle \varphi \rangle &= \langle \psi \rangle \langle \varphi \rangle, \\ \left\langle \frac{\partial \psi}{\partial t} \right\rangle &= \frac{\partial \langle \psi \rangle}{\partial t}, & \left\langle \frac{\partial \psi}{\partial x_i} \right\rangle &= \frac{\partial \langle \psi \rangle}{\partial x_i} \end{aligned}$$

- But in general

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



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

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

Treating  $\chi_d$  as a generalized function one can find

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

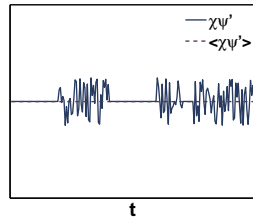
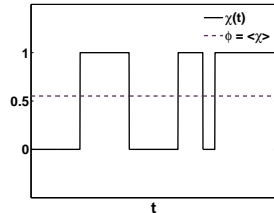
and justify the notation

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

The term  $\frac{\partial \chi_d}{\partial n}$  acts like a  $\delta$ -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  $\alpha$  in a multiphase flow one has

$$\frac{\partial \rho_\alpha}{\partial t} + \nabla \cdot \rho_\alpha \mathbf{v} = 0$$

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

in the interior, with the tensor of stresses

$$\mathbf{T}_\alpha = -p\mathbf{I} + \mu_\alpha [\nabla \mathbf{v} + (\nabla \mathbf{v})^T]$$

and the interfaces the jump conditions

$$\llbracket \rho_\alpha (\mathbf{v} - \mathbf{v}_S) \cdot \mathbf{n} \rrbracket = 0$$

$$\llbracket \rho_\alpha \mathbf{v} (\mathbf{v} - \mathbf{v}_S) \cdot \mathbf{n} - \mathbf{T}_\alpha \cdot \mathbf{n} \rrbracket = \sigma \kappa \mathbf{n}$$

$\rho_\alpha \dots$  density

$\mu_\alpha \dots$  viscosity

$f \dots$  volume force

$\mathbf{v}_S \dots$  interface  $\mathbf{v}$

$\mathbf{n} \dots$  normal vector

$\kappa \dots$  curvature

$\sigma \dots$  interfacial

tension

Exemplarily for the dispersed phase for the continuum equation

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

Multiply by  $\chi_d$  and decompose  $\mathbf{v} = \langle \mathbf{v} \rangle + \mathbf{v}'$ :

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

Rearrange by product rule, e.g.

$$\chi_d \frac{\partial \rho_d}{\partial t} = \frac{\partial \chi_d \rho_d}{\partial t} - \rho_d \frac{\partial \chi_d}{\partial t} = \frac{\partial \chi_d \rho_d}{\partial t} + \rho_d \mathbf{v}_s \cdot \nabla \chi_d$$

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

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

- Result: The averaged continuum equation for the dispersed phase

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

- Similar actions for the momentum equation deliver:

$$\begin{aligned} \frac{\partial \phi \rho_d \langle \mathbf{v} \rangle}{\partial t} + \nabla \cdot \phi \rho_d \langle \mathbf{v} \rangle \langle \mathbf{v} \rangle - \nabla \cdot \phi \mathbf{T}_d^* - \phi \rho_d \mathbf{f} &= \\ &= \langle [\rho_d \langle \mathbf{v} \rangle (\langle \mathbf{v} \rangle - \mathbf{v}_s) - \mathbf{T}_d^*] \cdot \nabla \chi_d \rangle. \end{aligned}$$

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

- Replace the subscript  $d$  by  $c$  and  $\phi$  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:

$$\langle [\rho_d \langle \mathbf{v} \rangle - \mathbf{v}_s]_d \cdot \nabla \chi_d \rangle = \langle \llbracket \rho_\alpha (\langle \mathbf{v} \rangle - \mathbf{v}_s) \cdot \mathbf{n} \rrbracket \rangle = 0$$

- For the momentum:

$$\begin{aligned} \langle [\rho_d \langle \mathbf{v} \rangle (\langle \mathbf{v} \rangle - \mathbf{v}_s) - \mathbf{T}_d^*] \cdot \nabla \chi_d \rangle = \\ \llbracket \rho_\alpha \langle \mathbf{v} \rangle (\langle \mathbf{v} \rangle - \mathbf{v}_s) \cdot \mathbf{n} - \mathbf{T}_\alpha^* \cdot \mathbf{n} \rrbracket = \sigma^* \kappa \mathbf{n} := \mathbf{M}_d^* \end{aligned}$$

where  $\sigma^*$  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

$$\begin{aligned} \frac{\partial \rho_c}{\partial t} + \nabla \rho_c \langle v \rangle &= \frac{\partial \phi \delta_\rho}{\partial t} + \nabla \phi \delta_\rho \langle v \rangle \\ \frac{\partial \rho_c \langle v \rangle}{\partial t} + \nabla \rho_c \langle v \rangle \langle v \rangle - \nabla T_c^* - \rho_c f &= \frac{\partial \phi \delta_\rho \langle v \rangle}{\partial t} + \nabla \phi \delta_\rho \langle v \rangle \langle v \rangle - \\ &\quad - \nabla \phi \delta_T^* - \phi \delta_\rho f + M_d^* + M_c^*. \end{aligned}$$



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

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

$$\begin{aligned} \frac{\partial \rho_c \langle \mathbf{v} \rangle}{\partial t} + \nabla \rho_c \langle \mathbf{v} \rangle \langle \mathbf{v} \rangle - \nabla T_c^* - \rho_c \mathbf{f} &= \frac{\partial \phi \delta_\rho \langle \mathbf{v} \rangle}{\partial t} + \nabla \phi \delta_\rho \langle \mathbf{v} \rangle \langle \mathbf{v} \rangle - \\ &\quad - \nabla \phi \delta T^* - \phi \delta_\rho \mathbf{f} + M_d^* + M_c^* \end{aligned}$$

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

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

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

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

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

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

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

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$$\frac{\partial \rho_c}{\partial t} + \nabla \rho_c \langle v \rangle = 0$$

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

- 0

$$0 = 0$$

## 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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For suggestions and questions please contact me



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