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

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• Stirring of two fluids
• Reynolds number $Re \sim 30,000$
• 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 simplified for simulations

- Two phases
- Phase interactions
- Inhomogeneous turbulent flow field

- 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 $f(t, x)$:

- e.g. time averaging:

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

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

- Properties

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

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

$$\langle \frac{\partial \psi}{\partial x_i} \rangle = \frac{\partial \langle \psi \rangle}{\partial x_i}.$$

- But in general

$$\langle \psi \varphi \rangle \neq \langle \psi \rangle \langle \varphi \rangle.$$
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 $\nu$ and the stresses $T$

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

but not for the densities $\rho = \langle \rho \rangle$. 
Phase-indicator function

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

Treating \( \chi_d \) 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)

\[ \langle \chi_d \psi \rangle = \phi \langle \psi \rangle \quad \text{and} \quad \langle \chi_d \psi' \rangle = 0 \]

\[ \langle \psi' \nabla \chi_d \rangle = 0 \]
(Boundary average)

which will be of major importance in the modelling.
For phase $\alpha$ in a multiphase flow one has

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

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

in the interior, with the tensor of stresses

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

and the interfaces the jump conditions

$$[[\rho_\alpha (\mathbf{v} - \mathbf{v}_s) \cdot n]] = 0$$

$$[[\rho_\alpha \mathbf{v} (\mathbf{v} - \mathbf{v}_s) \cdot n - T_\alpha \cdot n]] = \sigma \kappa n$$

$\rho_\alpha$ ... density
$\mu_\alpha$ ... viscosity
$\mathbf{f}$ ... volume force
$\mathbf{v}_s$ ... interface $\mathbf{v}$
$n$ ... normal vector
$\kappa$ ... curvature
$\sigma$ ... 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

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

Similar actions for the momentum equation deliver:

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

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 \( \phi \) 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:

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

- For the momentum:

\[
\langle [\rho_d\langle v \rangle(\langle v \rangle - v_s) - T^*_{dd}] \cdot \nabla \chi_d \rangle = \\
\langle [\rho_\alpha\langle v \rangle(\langle v \rangle - v_s) \cdot n - T^*_\alpha \cdot n] \rangle = \sigma^* \kappa n := M^*_d
\]

where \( \sigma^* \) is the turbulent interfacial tension.

- And for the equations corresponding to the continuous phase
Having introduced the symbols for the differences

\[ \delta \rho = \rho_c - \rho_d \quad \text{and} \quad \delta^* = \langle T_c \rangle - \langle T_d \rangle - \delta \rho \langle v'v' \rangle \]

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

\[
\begin{align*}
\frac{\partial \rho_c}{\partial t} + \nabla \rho_c \langle v \rangle &= \frac{\partial \phi \delta \rho}{\partial t} + \nabla \phi \delta \rho \langle v \rangle \\
\frac{\partial \rho_c \langle v \rangle}{\partial t} + \nabla \rho_c \langle v \rangle \langle v \rangle - \nabla T^*_c - \rho_c f &= \frac{\partial \phi \delta \rho \langle v \rangle}{\partial t} + \nabla \phi \delta \rho \langle v \rangle \langle v \rangle - \\
&- \nabla \phi \delta T^* - \phi \delta \rho f + M^*_d + M^*_c.
\end{align*}
\]
$T^*$ and $M^*$ have to be modelled

Then a population balance equation $P(\phi, \langle v \rangle, T^*) = 0$ closes the system:

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

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

$$- \nabla \phi \delta T^* - \phi \delta \rho f + M_d^* + M_c^*$$

$$0 = P(\phi, \langle v \rangle, T^*)$$
For the simulation we assumed that $\phi$ 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:

$$\begin{align*}
\frac{\partial \rho_c}{\partial t} + \nabla \rho_c \langle v \rangle &= \frac{\partial \phi \delta_\rho}{\partial t} + \nabla \phi \delta_\rho \langle v \rangle \\
\frac{\partial \rho_c \langle v \rangle}{\partial t} + \nabla \rho_c \langle v \rangle \langle v \rangle - \nabla T_c^* - \rho_c f &= \frac{\partial \phi \delta_\rho \langle v \rangle}{\partial t} + \nabla \phi \delta_\rho \langle v \rangle \langle v \rangle - \nabla \phi \delta_T^* - \phi \delta_\rho f + M_d^* + M_c^* \\
0 &= P(\phi, \langle v \rangle, T^*)
\end{align*}$$
For the simulation we assumed that $\phi$ 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:

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

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

$$0 = 0$$
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 $\delta \rho \to 0$.
- 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
