Modeling and Simulation of Dispersions in Turbulent Flows

- Bachelor Thesis -

Manuel Baumann

Diplomanden- und Doktorandenseminar Numerische Mathematik

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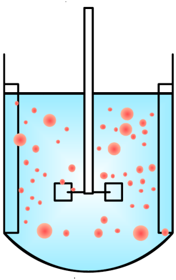
Table of Contents

Aim:

- Modeling and simulation of a dispersed phase during the mixing process in a stirrer



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- Model the dispersed phase by a Population-Balance Equation

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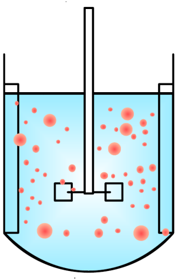

- Describe the flow behavior with the Navier-Stokes Equations
- Model the dispersed phase by a Population-Balance Equation

Books and articles

This work is based on the following books and articles:

A. J. Chorin and J. E. Marsden
A Mathematical Introduction to Fluid Mechanics
Springer-Verlag, New York/Berlin/Heidelberg/Tokyo, 1979

A. Gerslauer
Herleitung und Reduktion populationsdynamischer Modelle am Beispiel der Flüssig-Flüssig-Extraktion
VDI Verlage, Düsseldorf, 1999

M. Griebler, T. Dornseifer and T. Neunhoeffer
Numerical Simulation in Fluid Dynamics - A Practical Introduction
SIAM, Philadelphia, 1998

B.E. Launder and D.B. Spalding
The numerical computation of turbulent flows
Comp. Meth. in Appl. Mech. and Eng., 3:269–289, 1974

The Reynolds-Averaged-Navier-Stokes (RANS) Equations

The flow behavior of incompressible Newton fluids in turbulent flows can be described by the RANS Equations:

$$\frac{\partial}{\partial t}\vec{U} + (\vec{U}\cdot\nabla)\vec{U} + \nabla P + \frac{2}{3}\nabla k - \mathrm{div}(\nu^*(\nabla\vec{U} + \nabla\vec{U}^T)) = 0, \quad (1)$$

$$\mathrm{div}\ \vec{U} = 0. \quad (2)$$

The following physical quantities are introduced:

- $\vec{U} : \Omega \times T \to \mathbb{R}^{2,3}$ mean value of the velocity,
- $P : \Omega \times T \to \mathbb{R}$ mean value of the pressure,
- ν^* includes the turbulent kinematic viscosity.

To **close** this system, transport equations for the *turbulent kinetic energy* k and the *dissipation rate* ϵ are derived by the k-ϵ model.

Introduce the *number density function* $Q : \Omega_e \times \Omega \times [0, T_{end}] \to \mathbb{R}$, such that:

$$N_{drops}(t) = \int_{\Omega} \int_{\Omega_e} Q(d_p, \vec{x}, t)\, dd_p\, d\vec{x},$$

with the space of internal variables $\Omega_e = [0, d_{max}]$.

Population-Balance Equation (PBE)

A transport equation for the number density function Q is derived in [2]:

$$\frac{\partial Q}{\partial t} + \mathrm{div}(\vec{U} Q) - \mathrm{div}(\nu_T \nabla Q) = S. \qquad (3)$$

Characterize Q via its moments:

$$m^{(l)}(\vec{x},t) := \int_{-\infty}^{\infty} d_p^l \cdot Q(d_p,\vec{x},t)\; dd_p = \int_0^{d_{max}} d_p^l \cdot Q(d_p,\vec{x},t)\; dd_p,\, l \in \mathbb{N}_0$$

Integrate equation (3) and multiply by d_p^l leads to:

$$\frac{\partial}{\partial t} m^{(l)} + \mathrm{div}(\vec{U} m^{(l)}) - \mathrm{div}(\nu_T \nabla m^{(l)}) = S^{(l)}, \qquad l \in \mathbb{N}_0 \qquad \text{(3a)}$$

with the source term $S^{(l)}(d_p) := \int_0^{d_{max}} d_p^l \cdot S(d_p)\; dd_p$.

Since Q is unknown, use numerical quadrature in the internal space:

$$\int_0^{d_{max}} d_p^l \cdot Q(d_p,\vec{x},t)\; dd_p = \int_0^{d_{max}} d_p^l d\nu_{\vec{x},t}(d_p) \approx \sum_{\alpha=1}^{N} \omega_\alpha(\vec{x},t)\; \xi_\alpha^l(\vec{x},t).$$

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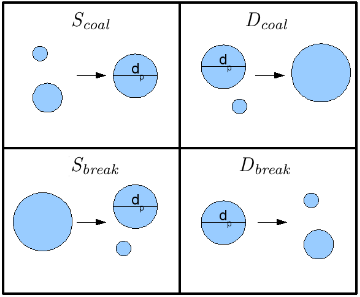
Modeling of the Source Terms $S^{(l)}$

The right-hand side of the PBE models drop breakage and drop coalescence:



$$S^{(l)}(d_p) = S^{(l)}_{break}(d_p) + S^{(l)}_{coal}(d_p) - D^{(l)}_{break}(d_p) - D^{(l)}_{coal}(d_p)$$

Modeling of the Source Terms $S^{(l)}$

Based on experimental investigations by Coulaloglou und Tavlarides the source terms are:

$$S_{break}(d_p) = \int_{d_p}^{d_{max}} n(d_p^{'})\beta(d_p, d_p^{'})\kappa(d_p^{'})Q(d_p^{'})\; dd_p^{'},$$

$$D_{break}(d_p) = \kappa(d_p)Q(d_p),$$

$$S_{coal}(d_p) = \frac{1}{2}\int_0^{d_p} \psi(d_p^{'}, d_p^{''})Q(d_p^{'})Q(d_p^{''})\; dd_p^{'}, \quad d_p^{''} := \sqrt[3]{d_p^3 - d_p^{'3}}$$

$$D_{coal}(d_p) = Q(d_p)\int_0^{\sqrt[3]{d_{max}^3 - d_p^3}} \psi(d_p, d_p^{\prime})Q(d_p^{\prime})\; dd_p.$$

- n - number of daughter drops,
- β - probability that the breakage of a drop $d_p^{\prime}$ leads to d_p,
- κ - probability of drop breakage,
- ψ - probability of coalescence of two drops.

Summary

The following system of equations is derived:

$$
\begin{aligned}
\frac{\partial}{\partial t}\vec{U} + (\vec{U}\cdot\nabla)\vec{U} + \nabla P + \frac{2}{3}\nabla k - \operatorname{div}(\nu^*(\nabla\vec{U} + \nabla\vec{U}^T)) &= 0, \\
\operatorname{div}\, \vec{U} &= 0, \\
\frac{\partial}{\partial t}k + \vec{U}\cdot\nabla k - \frac{\nu_T}{2}\|\nabla\vec{U} + \nabla\vec{U}^T\|_F^2 - \operatorname{div}(\nu_T\nabla k) + \epsilon &= 0, \\
\frac{\partial}{\partial t}\epsilon + \vec{U}\cdot\nabla\epsilon - \frac{c_1}{2}k\|\nabla\vec{U} + \nabla\vec{U}^T\|_F^2 - \operatorname{div}(\frac{c_\epsilon}{c_\mu}\nu_T\nabla\epsilon) + c_2\frac{\epsilon^2}{k} &= 0, \\
\frac{\partial}{\partial t}m^{(l)} + \operatorname{div}(\vec{U}m^{(l)}) - \operatorname{div}(\nu_T\nabla m^{(l)}) &= S^{(l)}.
\end{aligned}
$$

Note that $\nu_T = c_\mu \frac{k^2}{\epsilon}$ depends on time and space, and $\nu^* := \nu + \nu_T$.

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\frac{\partial}{\partial t}\epsilon + \vec{U}\cdot\nabla\epsilon - \frac{c_1}{2}k\|\nabla\vec{U} + \nabla\vec{U}^T\|_F^2 - \operatorname{div}(\frac{c_\epsilon}{c_\mu}\nu_T\nabla\epsilon) + c_2\frac{\epsilon^2}{k} &= 0,\\
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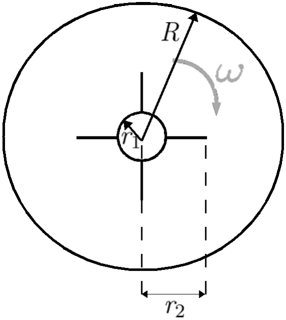
The numerical simulation is done for a simplified, two-dimensional stirrer:



The stirrer is described via:

- R - radius of the stirrer tank,
- r_1 - inner radius,
- r_2 - length of the stirrer baffles,
- ω - rotation speed.

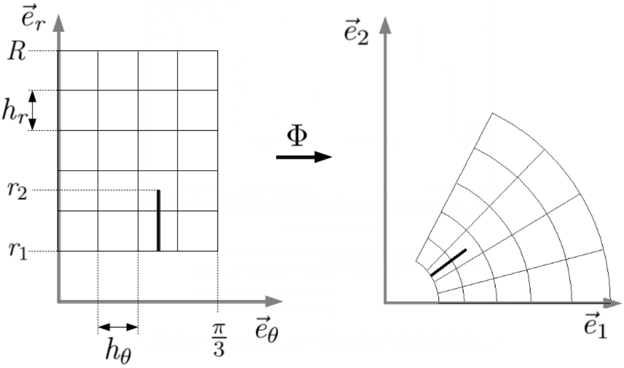
The geometry of the stirrer is described in polar coordinates.

In polar coordinates, the stirrer is a rectangular domain (left).

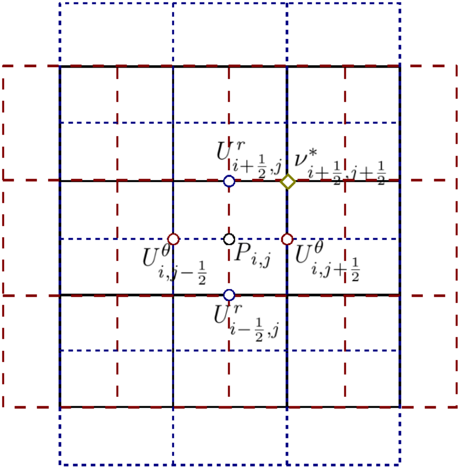
The coordinate transformation

$$\Phi : [r_1, R] \times [0, 2\pi) \rightarrow \mathbb{R}^2, \Phi(r, \theta) = \begin{bmatrix} r \cdot \cos\theta \\ r \cdot \sin\theta \end{bmatrix}$$

is used to represent the stirrer in Cartesian coordinates (right).



For the discretization, the usage of *staggered grids* is necessary:



Consider e.g. the transport equation for the *turbulent kinetic energy* k:

$$\frac{\partial}{\partial t}k + \underbrace{\vec{U}\cdot\nabla k - \mathrm{div}(\nu_T \nabla k)}_{=:R^k} - \frac{\nu_T}{2}\|\nabla\vec{U} + \nabla\vec{U}^T\|_F^2 + \epsilon = 0.$$

As a first step, all differential operators are expressed in polar coordinates:

$$\begin{aligned} R^k = \vec{U}\cdot\nabla k - \mathrm{div}(\nu_T \nabla k) &= \begin{bmatrix} U^r \\ U^\theta \end{bmatrix} \cdot \begin{bmatrix} \frac{\partial k}{\partial r} \\ \frac{1}{r}\frac{\partial k}{\partial \theta} \end{bmatrix} - \mathrm{div} \begin{bmatrix} \nu_T \frac{\partial k}{\partial r} \\ \nu_T \frac{1}{r}\frac{\partial k}{\partial \theta} \end{bmatrix} \\ &= \left(U^r \frac{\partial k}{\partial r} + U^\theta \frac{1}{r}\frac{\partial k}{\partial \theta} \right) - \frac{1}{r}\frac{\partial}{\partial r}\left(r\cdot\nu_T \frac{\partial k}{\partial r} \right) - \frac{1}{r}\frac{\partial}{\partial \theta}\left(\nu_T \frac{1}{r}\frac{\partial k}{\partial \theta} \right) \end{aligned}$$

A **finite differences** discretization of

$$R^k = \left(U^r \frac{\partial k}{\partial r} + U^\theta \frac{1}{r}\frac{\partial k}{\partial \theta}\right) - \frac{1}{r}\frac{\partial}{\partial r}\left(r \cdot \nu_T \frac{\partial k}{\partial r}\right) - \frac{1}{r}\frac{\partial}{\partial \theta}\left(\nu_T \frac{1}{r}\frac{\partial k}{\partial \theta}\right)$$

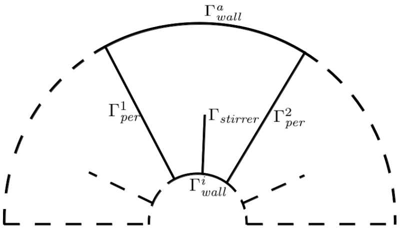
is given by:

$$\begin{aligned}
R^k_{i,j} \approx{} & \min(U^r_{i,j}, 0) \cdot \frac{k_{i+1,j} - k_{i,j}}{h_r} + \max(U^r_{i,j}, 0) \cdot \frac{k_{i,j} - k_{i-1,j}}{h_r} \\
& + \min(U^\theta_{i,j}, 0) \cdot \frac{1}{r_{i,j}} \frac{k_{i,j+1} - k_{i,j}}{h_\theta} + \max(U^\theta_{i,j}, 0) \cdot \frac{1}{r_{i,j}} \frac{k_{i,j} - k_{i,j-1}}{h_\theta} \\
& - \frac{1}{r_{i,j} \cdot h_r^2} \left(r_{i+\frac{1}{2},j} \cdot \nu_T^{i+\frac{1}{2},j} \cdot (k_{i+1,j} - k_{i,j}) - r_{i-\frac{1}{2},j} \cdot \nu_T^{i-\frac{1}{2},j} \cdot (k_{i,j} - k_{i-1,j}) \right) \\
& - \frac{1}{r_{i,j} \cdot h_\theta^2} \left(\frac{\nu_T^{i,j+\frac{1}{2}}}{r_{i,j+\frac{1}{2}}} (k_{i,j+1} - k_{i,j}) - \frac{\nu_T^{i,j-\frac{1}{2}}}{r_{i,j-\frac{1}{2}}} (k_{i,j} - k_{i,j-1}) \right).
\end{aligned}$$

The convection term is discretized using an **Upwind scheme**.

Boundary Conditions

Boundary conditions for one sixth of the stirrer:



- For the velocity:

$$U^r = \begin{cases} 0 & \text{on } \Gamma^i_{wall}, \\ 0 & \text{on } \Gamma^a_{wall}, \\ 0 & \text{on } \Gamma_{stirrer}, \end{cases} \qquad U^\theta = \begin{cases} \omega r_1 & \text{on } \Gamma^i_{wall}, \\ 0 & \text{on } \Gamma^a_{wall}, \\ \omega r & \text{on } \Gamma_{stirrer}. \end{cases}$$

- Use a specific *wall function* as Dirichlet values for k and ϵ.
- Use Neumann boundary conditions for the moments.

Time Integration

Assuming the RANS equation is discretized in space:

$$\frac{\partial}{\partial t}\vec{U} = \overbrace{-(\vec{U}\cdot\nabla)\vec{U} - \frac{2}{3}\nabla k + \mathrm{div}(\nu^*(\nabla\vec{U} + \nabla\vec{U}^T))}^{=:[F,G]^T} - \nabla P.$$

Then, a componentwise Euler-discretization is given by:

$$U_r^{(n+1)} = \overbrace{U_r^{(n)} + \delta t F^{(n)}}^{=:\tilde{F}^{(n)}} - \delta t \frac{\partial P^{(n+1)}}{\partial r},$$

$$U_\theta^{(n+1)} = \underbrace{U_\theta^{(n)} + \delta t G^{(n)}}_{=:\tilde{G}^{(n)}} - \delta t \frac{1}{r}\frac{\partial P^{(n+1)}}{\partial \theta}.$$

To guarantee a divergence-free velocity field, compute:

$$0 \stackrel{!}{=} \mathrm{div}\vec{U} = \mathrm{div}\begin{bmatrix} \tilde{F}^{(n)} - \delta t \frac{\partial P^{(n+1)}}{\partial r} \\ \tilde{G}^{(n)} - \delta t \frac{1}{r}\frac{\partial P^{(n+1)}}{\partial \theta} \end{bmatrix}.$$

This leads to the so-called *Pressure Poisson Equation (PPE)*:

$$\Delta P^{(n+1)} = \frac{1}{\delta t \cdot r}\left(\frac{\partial}{\partial r}(r \cdot \tilde{F}^{(n)}) + \frac{\partial \tilde{G}^{(n)}}{\partial \theta}\right) =: \eta^{(n)}$$

In one time step, one has to:

- solve the PPE $\Delta P^{(n+1)} = \eta^{(n)}$,
- compute corresponding velocity values,
- update the scalar values k, ϵ and $m^{(l)}$ using explicit Euler method.

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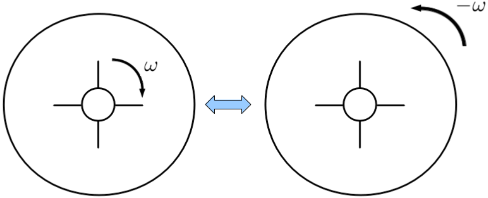
Model the movement of the stirring staff by the usage of rotating coordinates:



Expand the RANS equation by:

- the Coriolis force: $-2\,\vec{\omega} \times \vec{U}$,
- the Centrifugal force: $-\vec{\omega} \times (\vec{\omega} \times \vec{r})$,
- a time dependent term: $-\dot{\vec{\omega}} \times \vec{r}$.

$$\frac{\partial}{\partial t}\vec{U} = -(\vec{U}\cdot\nabla)\vec{U} - \frac{2}{3}\nabla k + \mathrm{div}(\nu^*(\nabla\vec{U} + \nabla\vec{U}^{\boldsymbol{T}})) - \nabla P - (2\,\vec{\omega} \times \vec{U}) - (\vec{\omega} \times (\vec{\omega} \times \vec{r})) - (\dot{\vec{\omega}} \times \vec{r}) \tag{1a}$$

Initialization, mesh generation, $t := 0$, $n := 0$

while $t < T_{end}$

1. Solve the PPE $\Delta P^{(n+1)} = \eta^{(n)}$
2. Calculate $\nabla P^{(n+1)}$
3. Calculate $\vec{U}^{(n+1)}$
4. Update k and ϵ by Euler time integration
5. Compute the source terms $S^{(l)}$ of the PBE
6. Update $m^{(l)}$ by Euler time integration
7. $t := t + \delta t$, $n := n + 1$

Visualization and transformation in non-rotating Cartesian coordinates

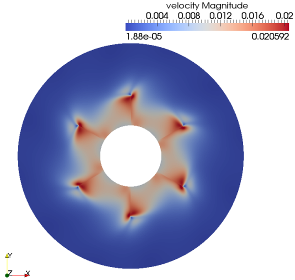
Numerical results:

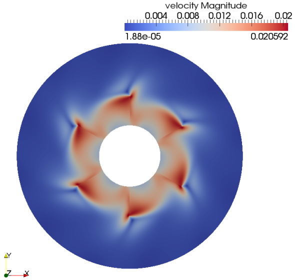
Parameter	Value
radius of the stirrer tank	$R = 0.075m$
inner radius	$r_1 = 0.02m$
length of the stirrer baffles	$r_2 = 0.04m$
rotation speed	$\omega = 0.5\frac{1}{s}$
size of time step	$\delta t = 10^{-6}s$
simulation time	$T_{end} = 0.0015s$
discretization of one segment	100 x 150

With a maximum velocity at the tip of the blade, $u_{tip} = 0.02\frac{m}{s}$, and a Reynolds number of

$$Re := \frac{\omega \cdot (2r_2)^2}{\nu} = 3.200.$$

at $Re = 3.200$


velocity Magnitude
0.004 0.008 0.012 0.016 0.02
1.88e-05
0.020592
Y
Z
X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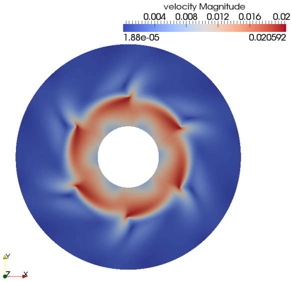
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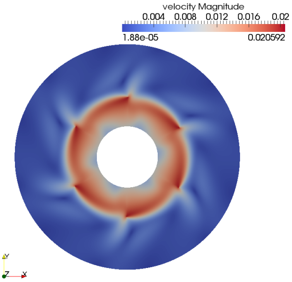
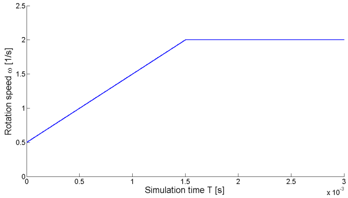
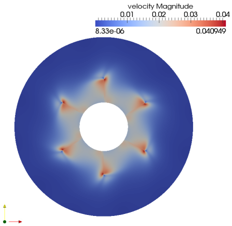
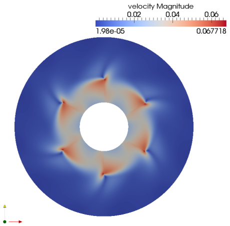

velocity Magnitude
0.004 0.008 0.012 0.016 0.02
1.88e-05
0.020592
Y
Z
X

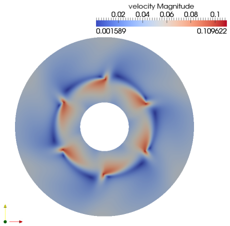
at $Re = 12.800$

For higher Reynolds numbers the rotation speed ω has to be increased in order to avoid numerical instability:









Summary and Outlook

- A mathematical description of a dispersed phase in turbulent flow is presented,
- the numerical simulation of the flow behavior in a two-dimensional stirrer shows good results,
- a larger time step is desirable,
- up to now, there is no stable implementation of the drop size distribution in a stirrer,
- the flow solver can be used as a control unit in future works.

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Thanks to Prof. Volker Mehrmann and Jan Heiland for the support!

Thanks for your attention!

Are there any questions / remarks ?