Forschungszentrum Karlsruhe
Technik und Umwelt

Institut für Reaktorsicherheit

Numerical Modeling of Multi-Phase Flows

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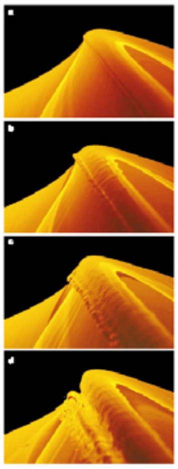
IP-EUROTRANS Internal Training Course ITC3:
"ADS thermal-hydraulics: system codes and CFD codes, models and experimental validation"
Louvain-La-Neuve, Belgium, March 21-24, 2007

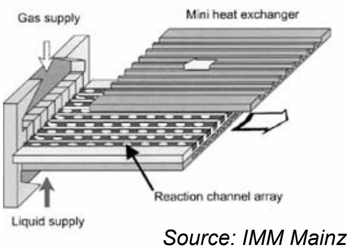
Examples of multiphase flow in nature

- Nature and environment
  - rain
  - sand storms
  - spreading of pollutants
  - CO_2 absorption in ocean
  - ...
  - sewage / waste water treatment plants



Examples of multiphase flows in industry

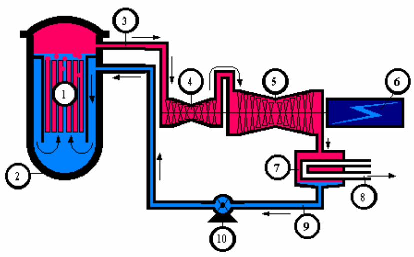
- Chemical process engineering
  - Transport of oil and its processing in refineries
  - Metal production and foundry industry
  - Production of chemicals in bubble columns
  - *Of interest is enhanced <u>mass transfer</u> capability of multiphase systems*

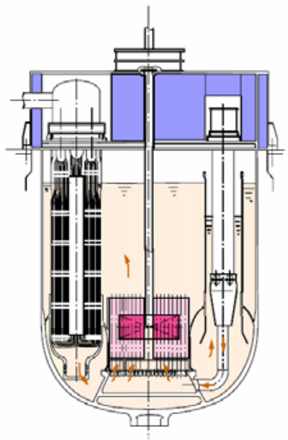


Source: IMM Mainz

Examples of multiphase flows in energy systems

- Combustion of liquid fuels
- Boiling water reactor (BWR)
- Pressurized water reactor (PWR)
- *Of interest is enhanced <u>heat transfer</u> capability of multiphase systems*





Scheme of an Accelerator Driven Transmutation System (ADS).

Goal of lecture

- Give an overview on common methods and models for numerical computation of multiphase-flows
- Provide understanding of the assumptions and limitations underlying the different models
- Support the selection of an appropriate model/method for a given multi-phase flow problem

Organization of Lecture

- Fundamental equations for multi-fluid flows
- Continuous field models
  - Homogenous model
  - Algebraic slip model
  - Two-fluid model
- Euler-Lagrange method
- Interface resolving simulation methods

Organization of Lecture

- **Fundamental equations for multi-fluid flows**
- Continuous field models
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Mathematical notation

Indices:
c = continuous phase
d = disperse phase
p = particle
1 = phase one (is always continuous)
2 = phase two (may be continuous or disperse)

Scalar	a	Unit vector	$\hat{\mathbf{e}}$
Vector	$\mathbf{a}$	Unit normal vector	$\hat{\mathbf{n}}$
Tensor	$\mathbb{A}$	Unit tangential vector	$\hat{\mathbf{t}}$
Transposed tensor	$\mathbb{A}^{\mathrm{T}}$	Unit tensor	$\mathbb{I}$

Mathematical notation

Scalar a

Vector $\mathbf{a} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}$

Tensor $\mathbb{A} = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix}$

Scalar product $\mathbf{a} \cdot \mathbf{b} = c$

Dyadic product $\mathbf{ab} = \mathbb{C}$

Double point product $\mathbb{A} : \mathbb{B} = c$

Nabla operator: $\nabla a = \mathbf{b}$

$\nabla \cdot \mathbf{a} = b$

$\nabla \cdot \mathbb{A} = \mathbf{b}$

Cartesian coordinates:

$$\nabla = \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix}$$

Governing equations for <u>single phase flow</u>

- Mass conservation in differential volume element gives

$$\boxed{\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{v} = 0}$$ and for ρ = constant $$\boxed{\nabla \cdot \mathbf{v} = 0}$$

- Momentum conservation equation for a Newtonian fluid

$$\underbrace{\frac{\mathrm{D}\rho\mathbf{v}}{\mathrm{D}t}}_{\text{inertia term}} = \underbrace{\frac{\partial \rho \mathbf{v}}{\partial t}}_{\text{unsteady term}} + \underbrace{\nabla \cdot \rho \mathbf{v}\mathbf{v}}_{\substack{\text{convective term} \\ \text{(non-linear!)}}} = \underbrace{-\nabla p}_{\substack{\text{pressure} \\ \text{gradient}}} + \underbrace{\nabla \cdot \mu \left[\nabla \mathbf{v} + (\nabla \mathbf{v})^{\mathrm{T}} \right]}_{\text{vicous term}} + \underbrace{\rho \mathbf{g}}_{\text{gravity}}$$

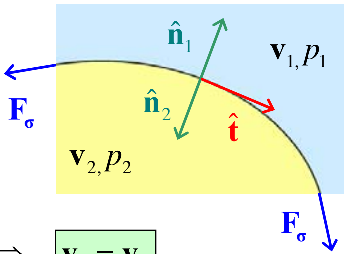
and for ρ = constant and μ = constant

$$\boxed{\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = -\frac{1}{\rho} \nabla p + \frac{\mu}{\rho} \nabla^2 \mathbf{v} + \mathbf{g}}$$

Navier Stokes equation

Boundary conditions at a fluid interface

- Assumptions
  - "functional interface" of zero thickness
  - no phase change / mass transfer



- Kinematic condition: $\boxed{\mathbf{v}_1 \cdot \hat{\mathbf{n}}_1 = \mathbf{v}_2 \cdot \hat{\mathbf{n}}_1}$
  - for two viscous fluids: $\boxed{\mathbf{v}_1 \cdot \hat{\mathbf{t}} = \mathbf{v}_2 \cdot \hat{\mathbf{t}}} \Rightarrow \boxed{\mathbf{v}_1 = \mathbf{v}_2}$
- Dynamic condition: $\boxed{-(p_1 - p_2)\hat{\mathbf{n}}_1 + (\mathbb{T}_1 - \mathbb{T}_2)\cdot\hat{\mathbf{n}}_1 = 2H\sigma\hat{\mathbf{n}}_1 + \nabla_s\sigma}$
  - σ = coefficient of surface tension
  - H = mean curvature of interface
  - $\mathbb{T}$ = viscous stress tensor $\mathbb{T}_k \equiv 2\mu_k \mathbb{D}_k$ with $\mathbb{D}_k \equiv \frac{1}{2}\left(\nabla\mathbf{v}_k + (\nabla\mathbf{v}_k)^{\mathrm{T}}\right)$

Dynamic boundary condition at a fluid interface

- Projection of dynamic b.c. in direction of unit normal vector

$$\boxed{-(p_1 - p_2) + (\mathbb{T}_1 - \mathbb{T}_2):\hat{\mathbf{n}}_1\hat{\mathbf{n}}_1 = 2H\sigma}$$

- Projection in direction of unit tangential vector

$$\boxed{(\mathbb{T}_1 - \mathbb{T}_2):\hat{\mathbf{n}}_1\hat{\mathbf{t}} = (\nabla_s\sigma)\cdot\hat{\mathbf{t}}}$$

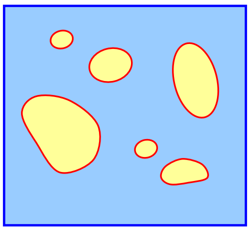
- <u>Free surface flows:</u> density and viscosity of phase 2 are neglected
  - for uniform coefficient of surface tension it follows

$$\boxed{p_1 - \mathbb{T}_1:\hat{\mathbf{n}}_1\hat{\mathbf{n}}_1 + 2H\sigma = p_2} \quad \text{(pressure } p_2 \text{ is constant)}$$

$$\boxed{\mathbb{T}_1:\hat{\mathbf{n}}_1\hat{\mathbf{t}} = 0} \quad \text{(zero tangential stress)}$$

Exact equations for flow of two immiscible fluids

$$\left.\begin{aligned}\frac{\partial \rho_1}{\partial t} + \nabla \cdot \rho_1 \mathbf{v}_1 = 0 \\ \frac{\partial \left(\rho_1 \mathbf{v}_1\right)}{\partial t} + \nabla \cdot \left(\rho_1 \mathbf{v}_1 \mathbf{v}_1\right) = -\nabla p_1 + \nabla \cdot \mathbb{T}_1 + \rho_1 \mathbf{g}\end{aligned}\right\} \mathbf{x} \in \Omega_1(t)$$



$$\left.\begin{aligned}\frac{\partial \rho_2}{\partial t} + \nabla \cdot \rho_2 \mathbf{v}_2 = 0 \\ \frac{\partial \left(\rho_2 \mathbf{v}_2\right)}{\partial t} + \nabla \cdot \left(\rho_2 \mathbf{v}_2 \mathbf{v}_2\right) = -\nabla p_2 + \nabla \cdot \mathbb{T}_2 + \rho_2 \mathbf{g}\end{aligned}\right\} \mathbf{x} \in \Omega_2(t)$$

$$\boxed{\Omega = \Omega_1(t) \cup \Omega_2(t) \neq \Omega(t)}$$

$$\boxed{\left.\begin{aligned}\mathbf{v}_1 = \mathbf{v}_2 = \mathbf{v}_{\mathrm{i}} \\ -\left(p_1 - p_2\right)\hat{\mathbf{n}}_1 + \left(\mathbb{T}_1 - \mathbb{T}_2\right) \cdot \hat{\mathbf{n}}_1 = 2H\sigma\hat{\mathbf{n}}_1 + \nabla_s \sigma\end{aligned}\right\} \mathbf{x} \in S_{\mathrm{i}}(t)}$$

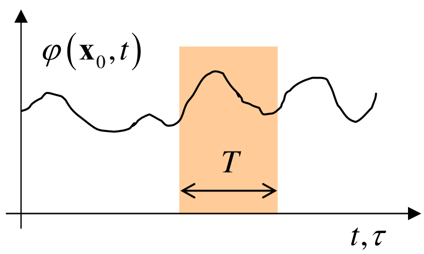
Interface: $S_{\mathrm{i}}(t) = \left(\partial\Omega_1 \cup \partial\Omega_2\right) / \partial\Omega$

Can be solved only for very special problems, see part on "Interface resolving simulation methods"

Averaging operations

- Types of averaging
  - Ensemble averaging or statistical averaging over a large number of realizations
  - Time averaging

$$\boxed{\overline{\varphi}^{T}\left(\mathbf{x}_0, t; T\right) = \frac{1}{T} \int_{t-T}^{t} \varphi\left(\mathbf{x}_0, \tau\right) \mathrm{d}\tau}$$



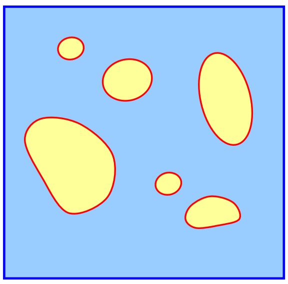
  - <u>Volume averaging</u> (here)
- All types of averaging yield formally similar equations

Basic idea of continuous field methods

- Instantaneous point of view
  - at any point in space there exists either phase 1 or 2

- Time averaged point of view
  - phases coexist and constitute **"interpenetrating continua"**

Mathematical description of phase distribution



Phase 1 in domain $\Omega_1(t)$

Phase 2 in domain $\Omega_2(t)$

Definition of two phase indicator functions:

$$X_k(\mathbf{x},t) \equiv \begin{cases} 1, & \text{if } \mathbf{x} \in \Omega_k(t) \\ 0, & \text{otherwise} \end{cases}$$

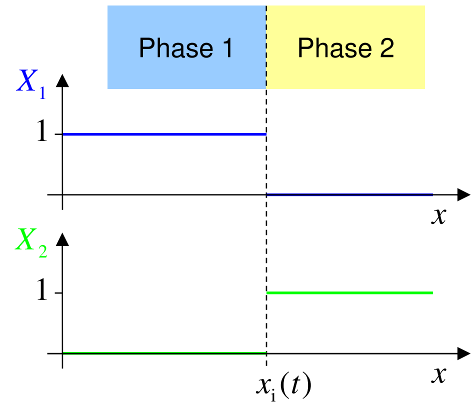
Properties:

$$X_1 + X_2 = 1$$

$$\frac{\mathrm{D}X_k}{\mathrm{D}t} = \frac{\partial X_k}{\partial t} + \mathbf{v}_\mathrm{i} \cdot \nabla X_k = 0$$

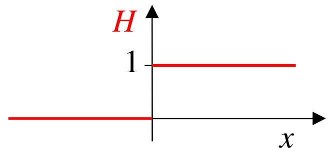
"Topological equation"

Phase indicator function in 1D



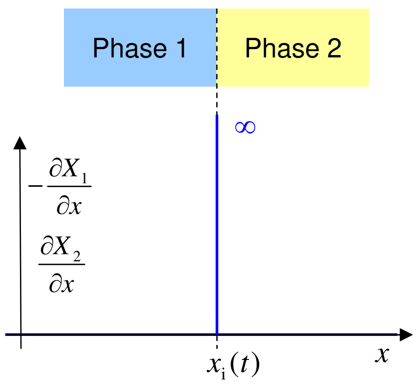
Heaviside function:

$$H(x) \equiv \begin{cases} 0, & x \le 0 \\ 1, & x > 0 \end{cases}$$



$$X_1(x,t) = 1 - H\left(x - x_i(t)\right)$$
$$X_2(x,t) = H\left(x - x_i(t)\right)$$

Gradient of phase indicator function



One-dimensional case:

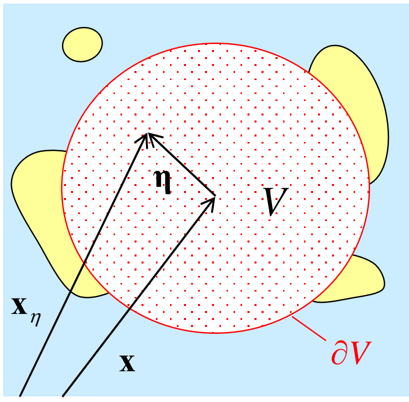
$$-\frac{\partial X_1}{\partial x} = \frac{\partial X_2}{\partial x} = \begin{cases} +\infty, & x = x_i \\ 0, & \text{otherwise} \end{cases}$$

Three-dimensional case: $\nabla X_k(\mathbf{x},t) = \hat{\mathbf{n}}_k \delta\left(\mathbf{x} - \mathbf{x}_i(t)\right)$

Dirac Delta function

Definitions for volume averaging

V	= averaging volume
∂V	= boundary of averaging volume
$\mathbf{x}$	= position vector to geometric center of V
$\mathbf{x}_\eta$	= position vector to arbitrary point within V
$\boldsymbol{\eta}$	= vector from $\mathbf{x}$ to $\mathbf{x}_\eta$



We do <u>not</u> make any assumption on the size or shape of V

Volume fractions of phases

- Volume occupied by phase k in V

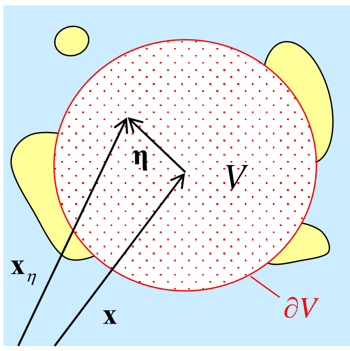
$$V_k(\mathbf{x},t;V) \equiv \iiint_V X_k(\mathbf{x}+\boldsymbol{\eta},t)\mathrm{d}\mathbf{x}_\eta$$

- Volume fraction of phase k in V

$$\alpha_k(\mathbf{x},t;V) \equiv \frac{1}{V}\iiint_V X_k(\mathbf{x}+\boldsymbol{\eta},t)\mathrm{d}\mathbf{x}_\eta = \frac{V_k}{V}$$

- Restriction for sum of volume fractions

$$\alpha_1 + \alpha_2 = 1$$



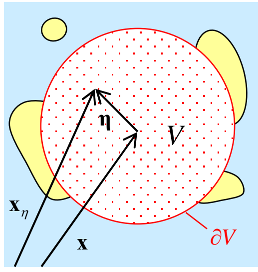
Definition of volume averaging operators

- Phase average of φ_k

$$\overline{\varphi_k}^{V}(\mathbf{x},t;V) \equiv \frac{1}{V}\iiint_V \varphi_k(\mathbf{x}+\boldsymbol{\eta},t) X_k(\mathbf{x}+\boldsymbol{\eta},t)\mathrm{d}\mathbf{x}_\eta$$

- Intrinsic phase average of φ_k

$$\overline{\varphi_k}^{V_k}(\mathbf{x},t;V) \equiv \frac{1}{V_k}\iiint_V \varphi_k(\mathbf{x}+\boldsymbol{\eta},t) X_k(\mathbf{x}+\boldsymbol{\eta},t)\mathrm{d}\mathbf{x}_\eta$$



- Relation between both averages:

$$\overline{\varphi_k}^{V} = \alpha_k \overline{\varphi_k}^{V_k}$$ ($\overline{\varphi_k}^{V_k}$ may be shortly written as $\overline{\varphi_k}^{k}$)

Derivation of volume averaged equations

- Multiplication of the mass and momentum conservation equation for each phase by respective phase indicator function
- Performing the average over the volume element V gives

$$\overline{X_k \frac{\partial \rho_k}{\partial t}}^{V} + \overline{X_k \nabla \cdot \rho_k \mathbf{v}_k}^{V} = 0$$

$$\overline{X_k \frac{\partial \rho_k \mathbf{v}_k}{\partial t}}^{V} + \overline{X_k \nabla \cdot \rho_k \mathbf{v}_k \mathbf{v}_k}^{V} = -\overline{X_k \nabla p_k}^{V} + \overline{X_k \nabla \cdot \mathbb{T}_k}^{V} + \overline{X_k \rho_k \mathbf{g}}^{V}$$

- Problem: Time derivative and Nabla operator do not commute with volume averaging operator!

Gauß and Leibniz rules for volume averaging

- Gauß rule for volume averaging

$$\overline{X_k \nabla \varphi_k}^V = \nabla \overline{X_k \varphi_k}^V - \overline{\varphi_k \nabla X_k}^V = \nabla \overline{X_k \varphi_k}^V - \frac{1}{V} \iint_{S_\mathrm{i} \cap V} \hat{\mathbf{n}}_k \varphi_{k\mathrm{i}} (\mathbf{x} + \boldsymbol{\eta}, t) \mathrm{d}S$$

  - here $S_\mathrm{i} \cap V$ is the surface forming the interface within V
  - and $\varphi_{k\mathrm{i}}$ is the value of φ at the k-side of the interface

- Leibniz rule for volume averaging

$$\overline{X_k \frac{\partial \varphi_k}{\partial t}}^V = \frac{\partial}{\partial t} \overline{X_k \varphi_k}^V - \overline{\varphi_k \frac{\partial X_k}{\partial t}}^V = \frac{\partial}{\partial t} \overline{X_k \varphi_k}^V + \overline{\varphi_{k\mathrm{i}} \mathbf{v}_\mathrm{i} \cdot \nabla X_k}^V$$
$$= \frac{\partial}{\partial t} \overline{X_k \varphi_k}^V + \frac{1}{V} \iint_{S_\mathrm{i} \cap V} \hat{\mathbf{n}}_k \cdot \mathbf{v}_\mathrm{i} \varphi_{k\mathrm{i}} \mathrm{d}s$$

  - here $\mathbf{v}_\mathrm{i}$ is the velocity of the interface

Volume averaged continuity equation

$$\overline{X_k \frac{\partial \rho_k}{\partial t}}^V + \overline{X_k \nabla \cdot \rho_k \mathbf{v}_k}^V = 0$$

Use of Gauß and Leibniz rule gives:

$$\frac{\partial (\alpha_k \rho_k)}{\partial t} + \nabla \cdot \alpha_k \rho_k \overline{\mathbf{v}_k}^{V_k} = \frac{1}{V} \iint_{S_\mathrm{i} \cap V} \hat{\mathbf{n}}_k \cdot \left(\mathbf{v}_\mathrm{i} - \mathbf{v}_{k\mathrm{i}} \right) \rho_k \mathrm{d}S \equiv \Gamma_k$$

Γ_k = mass transfer across the interface due to phase change

Jump condition: $\Gamma_1 + \Gamma_2 = 0$ No phase change: $\Gamma_1 = \Gamma_2 = 0$

$$\Rightarrow \boxed{\frac{\partial (\alpha_k \rho_k)}{\partial t} + \nabla \cdot \alpha_k \rho_k \overline{\mathbf{v}_k}^{V_k} = 0}$$

Volume averaged momentum equation

Assumptions: incompressible fluids, no phase change

$$\frac{\partial \alpha_k \rho_k \overline{\mathbf{v}_k}^{V_k}}{\partial t} + \nabla \cdot \alpha_k \rho_k \overline{\mathbf{v}_k \mathbf{v}_k}^{V_k} = -\nabla \alpha_k \overline{p_k}^{V_k} + \alpha_k \rho_k \mathbf{g} + \nabla \cdot \alpha_k \overline{\mathbb{T}_k}^{V_k} + \mathbf{M}_k$$

$\mathbf{M}_k$ = momentum transfer term across the interface

$$\mathbf{M}_k = -\overline{\left(-p_k \mathbb{I} + \mathbb{T}_k\right) \cdot \nabla X_k}^{V}$$

$$\nabla X_k(\mathbf{x},t) = \hat{\mathbf{n}}_k \delta\left(\mathbf{x} - \mathbf{x}_\mathrm{i}(t)\right)$$

$$\mathbf{M}_k = -\frac{1}{V}\iiint_V \left(-p_k \mathbb{I} + \mathbb{T}_k\right) \cdot \hat{\mathbf{n}}_k \delta\left(\mathbf{x} - \mathbf{x}_\mathrm{i}(t)\right) \mathrm{d}\mathbf{x}_\eta = -\frac{1}{V} \boxed{\iint_{S_\mathrm{i} \cap \mathrm{V}} \left(-p_k \mathbb{I} + \mathbb{T}_k\right) \cdot \hat{\mathbf{n}}_k \mathrm{d}S}$$

Integral of pressure and viscous stresses over that part of the interface that is within the averaging volume V

Coupling of the two momentum equations

$$\frac{\partial \alpha_1 \rho_1 \overline{\mathbf{v}_1}^{V_1}}{\partial t} + \nabla \cdot \alpha_1 \rho_1 \overline{\mathbf{v}_1 \mathbf{v}_1}^{V_1} = -\nabla \alpha_1 \overline{p_1}^{V_1} + \alpha_1 \rho_1 \mathbf{g} + \nabla \cdot \alpha_1 \overline{\mathbb{T}_1}^{V_1} + \mathbf{M}_1$$

$$\frac{\partial \alpha_2 \rho_2 \overline{\mathbf{v}_2}^{V_2}}{\partial t} + \nabla \cdot \alpha_2 \rho_2 \overline{\mathbf{v}_2 \mathbf{v}_2}^{V_2} = -\nabla \alpha_2 \overline{p_2}^{V_2} + \alpha_2 \rho_2 \mathbf{g} + \nabla \cdot \alpha_2 \overline{\mathbb{T}_2}^{V_2} + \mathbf{M}_2$$

Momentum jump condition at the interface:

$$\mathbf{M}_1 + \mathbf{M}_2 = \frac{1}{V} \iint_{S_\mathrm{i} \cap V} \left(\sigma H \hat{\mathbf{n}}_1 + \nabla_s \sigma\right) \mathrm{d}S$$

- Derived from volume averaging of dynamic b.c. at interface
- Phase momentum equations are coupled by jump condition

Turbulence and subgrid stress tensor

- Decomposition of local velocity
  - spatial fluctuation = local value – spatial mean

$$\boxed{\mathbf{v}_k' = \mathbf{v}_k - \overline{\mathbf{v}_k}^k}$$

- The non-linear convective term then yields

$$\alpha_k \rho_k \overline{\mathbf{v}_k \mathbf{v}_k}^k = \alpha_k \rho_k \overline{\mathbf{v}_k}^k \overline{\mathbf{v}_k}^k - \alpha_k \mathbb{T}_k^{sgs} \quad \text{where}$$

$$-\mathbb{T}_k^{sgs} \equiv \underbrace{\rho_k \left(\overline{\overline{\mathbf{v}_k}^k \overline{\mathbf{v}_k}^k}^k - \overline{\mathbf{v}_k}^k \overline{\mathbf{v}_k}^k \right)}_{\mathbb{L}_k} + \underbrace{\rho_k \left(\overline{\overline{\mathbf{v}_k}^k \mathbf{v}_k'}^k + \overline{\mathbf{v}_k' \overline{\mathbf{v}_k}^k}^k \right)}_{\mathbb{C}_k} + \underbrace{\rho_k \overline{\mathbf{v}_k' \mathbf{v}_k'}^k}_{\mathbb{R}_k}$$

  - $\mathbb{T}_k^{sgs}$ = subgrid stress tensor
  - $\mathbb{R}_k$ = subgrid-stress Reynolds stress tensor

Large eddy simulation

- Similarly, time averaging yields turbulent Reynolds stress tensor
  - statistical modeling of turbulence (e.g. k-ε turbulence model)

Closure problem

Equations	#
Mass conservation phase 1	1
Mass conservation phase 2	1
Momentum conservation phase 1	3
Momentum conservation phase 2	3
Constraint on volume fractions	1
Momentum jump condition	3
Total	**12**

Unknowns	#
α_1, α_2	2
$\overline{\mathbf{v}_1}^1, \overline{\mathbf{v}_2}^2$	6
$\overline{p_1}^1, \overline{p_2}^2$	2
$\mathbf{M}_1, \mathbf{M}_2$	6
$\mathbb{T}_1^{sgs}, \mathbb{T}_2^{sgs}$	12
Total	**28**

Organization of Lecture

- Fundamental equations for multi-fluid flows
- **Continuous field models**
  - Homogenous model
  - Algebraic slip model
  - Two-fluid model
- Euler-Lagrange method
- Interface resolving simulation methods

Continuous field models: closure problem

Equations	#
Mass conservation phase 1	1
Mass conservation phase 2	1
Momentum conservation phase 1	3
Momentum conservation phase 2	3
Constraint on volume fractions	1
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Total	**12**

Unknowns	#
α_1, α_2	2
$\overline{\mathbf{v}_1}^1, \overline{\mathbf{v}_2}^2$	6
$\overline{p_1}^1, \overline{p_2}^2$	2
$\mathbf{M}_1, \mathbf{M}_2$	6
$\mathbb{T}_1^{sgs}, \mathbb{T}_2^{sgs}$	12
Total	**28**

Continuous field models: closure assumptions

Equations	#
Mass conservation phase 1	1
Mass conservation phase 2	1
Momentum conservation phase 1	3
Momentum conservation phase 2	3
Constraint on volume fractions	1
Momentum jump condition	3
Total	**12**

Unknowns	#
α_1, α_2	2
$\overline{\mathbf{v}_1}^1, \overline{\mathbf{v}_2}^2$	6
$\overline{p_1}^1 = \overline{p_2}^2 = p$	1
$\mathbf{M}_1, \mathbf{M}_2$	6
$\mathbb{T}_1^{sgs} = \mathbb{T}_2^{sgs} = 0$	0
Total	**15**

Continuous field models: closure strategies

- Three constitutive closure relations are required
- Three strategies with different complexity:

1.) Homogeneous model (HM)

- Phases are in mechanical equilibrium: $\overline{\mathbf{v}_2}^{V_2} = \overline{\mathbf{v}_1}^{V_1}$

2.) Algebraic slip model (ASM)

- Algebraic relation for $\mathbf{v}_r = \overline{\mathbf{v}_2}^{V_2} - \overline{\mathbf{v}_1}^{V_1}$

3.) Two-fluid model (Euler-Euler model)

- Constitutive equation for $\mathbf{M}_1$

Homogeneous model (HM)

- In the homogeneous model it is assumed that both phases are in "mechanical equilibrium" and move with the same velocity
- The closure relation is therefore

$$\boxed{\overline{\mathbf{v}_2}^{V_2} = \overline{\mathbf{v}_1}^{V_1}} \quad \text{or} \quad \boxed{\mathbf{v}_\mathbf{r} \equiv \overline{\mathbf{v}_2}^{V_2} - \overline{\mathbf{v}_1}^{V_1} = 0}$$

- In the HM only one momentum equation is solved, which is the momentum equation for the two-phase mixture
- This mixture momentum equation is obtained by summing up the momentum equations of the individual phases

Set of equations of homogeneous model

- Mass conservation of both phases

$$\boxed{\frac{\partial \alpha_1}{\partial t} + \nabla \cdot \alpha_1 \mathbf{v}_\mathrm{m} = 0} \quad \text{and} \quad \boxed{\nabla \cdot \mathbf{v}_\mathrm{m} = 0}$$

- Mixture momentum equation

$$\boxed{\frac{\partial \rho_\mathrm{m} \mathbf{v}_\mathrm{m}}{\partial t} + \nabla \cdot \rho_\mathrm{m} \mathbf{v}_\mathrm{m} \mathbf{v}_\mathrm{m} = -\nabla p + \rho_\mathrm{m} \mathbf{g} + \nabla \cdot \mu_\mathrm{m} \left(\nabla \mathbf{v}_\mathrm{m} + \nabla \mathbf{v}_\mathrm{m}^{\mathrm{T}} \right) + \frac{1}{V} \iint_{S_\mathrm{i} \cap V} \sigma H \hat{\mathbf{n}}_1 \, \mathrm{d}s}$$

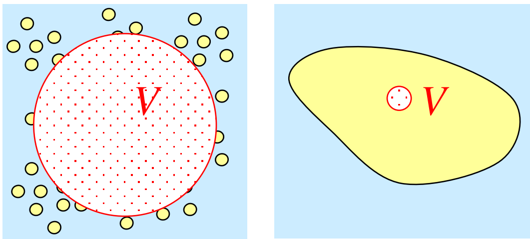
- Definitions of the mixture quantities

$$\boxed{\mathbf{v}_\mathrm{m} \equiv \frac{\alpha_1 \rho_1 \overline{\mathbf{v}_1}^{V_1} + \alpha_2 \rho_2 \overline{\mathbf{v}_2}^{V_2}}{\alpha_1 \rho_1 + \alpha_2 \rho_2}} \quad \boxed{\rho_\mathrm{m} \equiv \alpha_1 \rho_1 + \alpha_2 \rho_2} \quad \boxed{\mu_\mathrm{m} \equiv \alpha_1 \mu_1 + \alpha_2 \mu_2}$$

Applicability of homogeneous model

The assumption of mechanical equilibrium is reasonable for two remarkably different flow regimes:

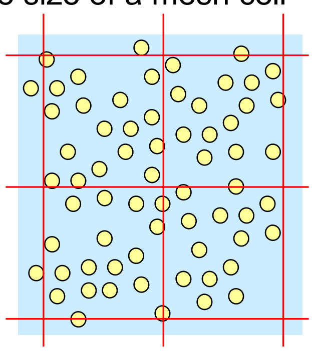
1. Phase 2 is finely dispersed in phase 1
2. Phase 1 and 2 are well separated



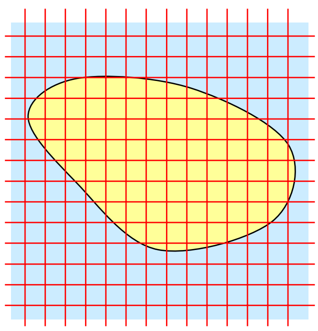
Fine dispersed or well separated depends on the size of the particle and the size of the averaging volume V

Applicability of homogeneous model

The size of the averaging volume V is usually related with the size of a mesh cell



In almost all cells it is $0 < \alpha_1 < 1$



In almost all cells it is either $\alpha_1=0$ or $\alpha_1=1$

Homogeneous model for disperse flow

- Mechanical equilibrium requires the relative velocity U_r to be very small
- Impact of forces on relative velocity U_r
  - Increase of U_r due to inertial forces F_I (acceleration / deceleration)
  - Increase of U_r due to buoyancy forces F_B
  - Decrease of U_r due to viscous forces F_V
- Ratios of these forces

$$\boxed{\frac{F_I}{F_V} = \frac{\rho_c d_{eq} U_r}{\mu_c} = Re_p} \Rightarrow \boxed{Re_p < 1}$$

$$\boxed{\frac{F_B}{F_V} = \frac{g \Delta \rho d_{eq}^2}{\mu_c V_r} = \frac{3}{4} Re_p C_D} \quad \boxed{C_{D,\,Stokes} = \frac{24}{Re_p}} \Rightarrow \boxed{\frac{F_B}{F_V} = 18} \Rightarrow$$

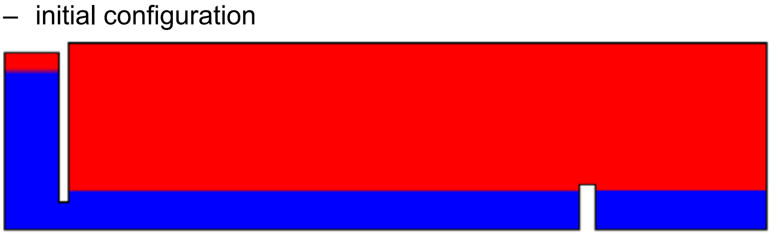
HM not applicable for buoyant flows!

Homogeneous model for disperse flow

- For a disperse flow the name homogeneous model is a little misleading because the HM does not assume that the disperse phase is homogeneously distributed
- Instead the phase distribution may be non-uniform and may change in time
- The homogeneous model does not make any assumption for the size or shape of bubbles and drops
- The technical relevance and applicability of the homogeneous model for disperse flow is very limited

Application of the HM to separate flow

- Example: Standard benchmark problem
  - initial configuration



- Computations with CFX 5.5
  - "free surface model" without surface tension
  - investigation of grid type (structured/unstructured)
  - investigation of spatial and temporal discretization schemes

Source: F. Menter, CFX Germany

Example application of the HM to separate flow

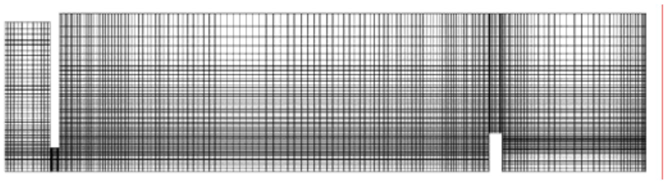
$$\alpha_1 = 1, \quad \alpha_2 = 0 \quad \Rightarrow \quad \rho_{\mathrm{m}} = \rho_1, \quad \mu_{\mathrm{m}} = \mu_1, \quad \mathbf{v}_{\mathrm{m}} = \overline{\mathbf{v}_1}^{V_1}$$

$$\frac{\partial \rho_1 \overline{\mathbf{v}_1}^{V_1}}{\partial t} + \nabla \cdot \rho_1 \overline{\mathbf{v}_1}^{V_1} \overline{\mathbf{v}_1}^{V_1} = -\nabla p + \rho_1 \mathbf{g} + \nabla \cdot \mu_1 \left(\nabla \overline{\mathbf{v}_1}^{V_1} + \left(\nabla \overline{\mathbf{v}_1}^{V_1} \right)^{\mathrm{T}} \right)$$

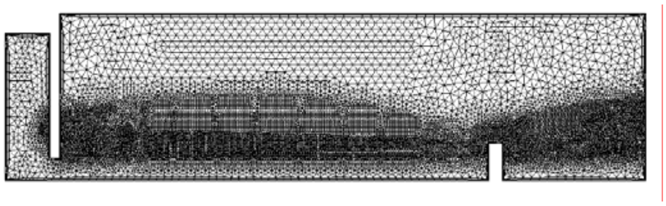
$$\alpha_1 = 0, \quad \alpha_2 = 1 \quad \Rightarrow \quad \rho_{\mathrm{m}} = \rho_2, \quad \mu_{\mathrm{m}} = \mu_2, \quad \mathbf{v}_{\mathrm{m}} = \overline{\mathbf{v}_2}^{V_2}$$

$$\frac{\partial \rho_2 \overline{\mathbf{v}_2}^{V_2}}{\partial t} + \nabla \cdot \rho_2 \overline{\mathbf{v}_2}^{V_2} \overline{\mathbf{v}_2}^{V_2} = -\nabla p + \rho_2 \mathbf{g} + \nabla \cdot \mu_2 \left(\nabla \overline{\mathbf{v}_2}^{V_2} + \left(\nabla \overline{\mathbf{v}_2}^{V_2} \right)^{\mathrm{T}} \right)$$

Mesh



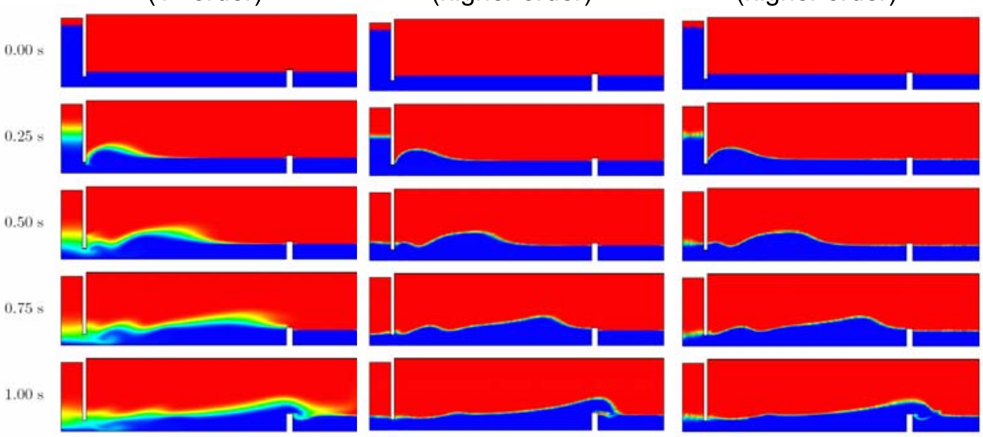
Structured quadrilateral mesh with 19010 cells



Unstructured triangular mesh with 32024 nodes

Results

Structured grid upwind + backward Euler (1^{st} order)	Structured grid high resolution scheme (higher order)	Unstructured grid high resolution scheme (higher order)



Organization of Lecture

- Fundamental equations for multi-fluid flows
- Continuous field models
  - Homogenous model
  - **Algebraic slip model**
  - Two-fluid model
- Euler-Lagrange method
- Interface resolving simulation methods

Algebraic slip model

Other names:
- Diffusion model
- Mixture model

Related model:
- Drift flux model

- Constitutive equation of the algebraic slip r
  - it is assumed that the relative velocity between
    (slip velocity) can be approximated by an algeb

$$\boxed{\mathbf{v}_\mathrm{r} = \mathbf{v}_\mathrm{r}(\rho_1, \rho_2, \mu_1, \mu_2, \sigma, \alpha_1, \mathbf{v}_\mathrm{m}, \ldots)}$$

  - This assumption is only meaningful for disperse flow
  - The homogeneous model is a special case of the ASM $(\mathbf{v}_\mathrm{r} = 0)$
  - The surface tension force is usually neglected

$$\frac{\partial \rho_\mathrm{m}}{\partial t} + \nabla \cdot \rho_\mathrm{m} \mathbf{v}_\mathrm{m} = 0 \qquad \frac{\partial \alpha_2 \rho_2}{\partial t} + \nabla \cdot \alpha_2 \rho_2 \mathbf{v}_\mathrm{m} = \boxed{\nabla \cdot \frac{\alpha_1 \alpha_2 \rho_1 \rho_2}{\rho_\mathrm{m}} \mathbf{v}_\mathrm{r}}$$

Extra term as compared to HM

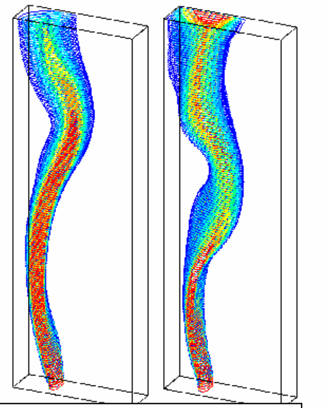
$$\frac{\partial \rho_\mathrm{m} \mathbf{v}_\mathrm{m}}{\partial t} + \nabla \cdot \rho_\mathrm{m} \mathbf{v}_\mathrm{m} \mathbf{v}_\mathrm{m} = -\nabla p_\mathrm{m} + \rho_\mathrm{m} \mathbf{g} + \nabla \cdot \mu_\mathrm{m} \left(\nabla \mathbf{v}_\mathrm{m} + \left(\nabla \mathbf{v}_\mathrm{m} \right)^\mathrm{T} \right)$$

Example: The flow in a flat bubble column

- Flat bubble column
  - Width 50 cm, depth 8 cm, height 150 cm
  - Air bubbles are injected in water
- Modeling of relative velocity

$$\boxed{\mathbf{v}_r = (0, 0, 20\,\mathrm{cm/s})^T = \mathrm{constant}}$$

  - Rise velocity is modeled independent of bubble size
  - Approach is valid only for bubbles of certain size and for mono-disperse flow (no coalescence / breakup)
  - Swarm effects are not taken into account



Computed instantaneous gas volume fraction

Source: Sokolichin & Eigenberger, Chemical Engineering Science 54 (1999) 2273-2284

Organization of Lecture

- Fundamental equations for multi-fluid flows
- Continuous field models
  - Homogenous model
  - Algebraic slip model
  - **Two-fluid model**
- Euler-Lagrange method
- Interface resolving simulation methods

The two-fluid model (Euler-Euler model)

Set of equations of the two-fluid model:

$$\frac{\partial \alpha_1 \rho_1 \overline{\mathbf{v}_1}^{V_1}}{\partial t} + \nabla\cdot\alpha_1\rho_1 \overline{\mathbf{v}_1}^{V_1}\overline{\mathbf{v}_1}^{V_1} = -\nabla\alpha_1 p + \nabla\cdot\alpha_1\mu_1\left(\nabla\overline{\mathbf{v}_1}^{V_1} + \left(\nabla\overline{\mathbf{v}_1}^{V_1}\right)^{\mathrm{T}}\right) + \alpha_1\rho_1\mathbf{g} + \mathbf{M}_1$$

$$\frac{\partial \alpha_2 \rho_2 \overline{\mathbf{v}_2}^{V_2}}{\partial t} + \nabla\cdot\alpha_2\rho_2 \overline{\mathbf{v}_2}^{V_2}\overline{\mathbf{v}_2}^{V_2} = -\nabla\alpha_2 p + \nabla\cdot\alpha_2\mu_2\left(\nabla\overline{\mathbf{v}_2}^{V_2} + \left(\nabla\overline{\mathbf{v}_2}^{V_2}\right)^{\mathrm{T}}\right) + \alpha_2\rho_2\mathbf{g} + \mathbf{M}_2$$

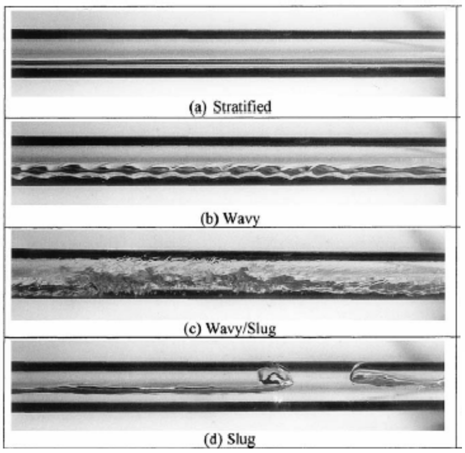
$$\frac{\partial \alpha_1\rho_1}{\partial t} + \nabla\cdot\alpha_1\rho_1\overline{\mathbf{v}_1}^{V_1} = 0 \qquad \frac{\partial \alpha_2\rho_2}{\partial t} + \nabla\cdot\alpha_2\rho_2\overline{\mathbf{v}_2}^{V_2} = 0 \qquad \mathbf{M}_1 + \mathbf{M}_2 = \frac{1}{V}\iint_{S_i\cap V}\sigma H\hat{\mathbf{n}}_1\mathrm{d}S$$

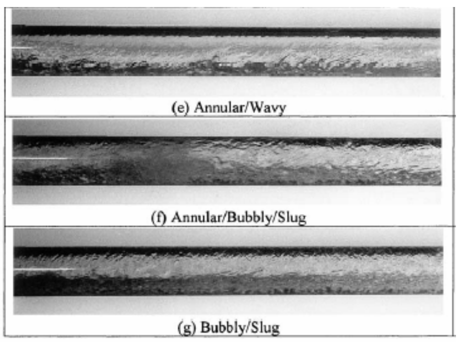
Closure assumption of the two-fluid model:

Constitutive equation for momentum transfer term $\mathbf{M}_1$

$$\mathbf{M}_1 = -\frac{1}{V}\iint_{S_i\cap V}\left[-p_1\mathbb{I} + \mu_1\left(\nabla\mathbf{v}_1 + \left(\nabla\mathbf{v}_1\right)^{\mathrm{T}}\right)\right]\cdot\hat{\mathbf{n}}_1\mathrm{d}S = \mathbf{M}_1(\rho_1,\rho_2,\mu_1,\mu_2,\sigma,\alpha_1,\overline{\mathbf{v}_1}^{V_1},\overline{\mathbf{v}_2}^{V_2},\ldots)$$

Photographs of air-water flow in a horizontal pipe





$$\mathbf{M}_1 = -\frac{1}{V}\iint_{S_i\cap V}\left[-p_1\mathbb{I} + \mu_1\left(\nabla\mathbf{v}_1 + \left(\nabla\mathbf{v}_1\right)^{\mathrm{T}}\right)\right]\cdot\hat{\mathbf{n}}_1\mathrm{d}S$$

Source: *Kim & Ghajar, Exp Therm Fluid Sci 25 (2002)*

Interfacial momentum transfer depends on the flow regime!

The momentum transfer term for a particle

For a particle (bubble, drop, rigid particle) the momentum transfer term is related to the force on particle surface

$$\mathbf{M}_1 = -\frac{1}{V}\iint_{S_\mathrm{i}\cap V}\left[-p_1\mathbb{I} + \mu_1\left(\nabla\mathbf{v}_1 + (\nabla\mathbf{v}_1)^\mathrm{T}\right)\right]\cdot\hat{\mathbf{n}}_1\mathrm{d}S = -\frac{1}{V}\iint_{S_\mathrm{i}\cap V}\left(-p_1\mathbb{I} + 2\mu_1\mathbb{D}_1\right)\cdot\hat{\mathbf{n}}_1\mathrm{d}S$$

$$\mathbf{F}_\text{surface} = \oiint_{\mathcal{A}_\mathrm{P}}\left(-p_1\mathbb{I} + 2\mu_1\mathbb{D}_1\right)\cdot\hat{\mathbf{n}}_1\mathrm{d}S$$

Important difference:

The integral in $\mathbf{M}_1$ is over that part of the interface that is within the averaging volume V,

while the integral in $\mathbf{F}_\text{surface}$ is over the entire particle surface

The force on a particle immersed in a fluid

- Newton's second law: $\rho_\mathrm{p}\mathcal{V}_\mathrm{p}\dfrac{\mathrm{d}\mathbf{V}_\mathrm{p}}{\mathrm{d}t} = \mathbf{F}_\Sigma = \mathbf{F}_\text{body} + \mathbf{F}_\text{surface}$

$\mathcal{V}_\mathrm{p}$ = volume of particle

$\mathbf{V}_\mathrm{p}$ = translational velocity of center-of-mass of particle

$$\mathbf{F}_\text{surface} = \oiint_{\mathcal{A}_\mathrm{P}}\left(-p_1\mathbb{I} + \mathbb{T}_1\right)\cdot\hat{\mathbf{n}}_1\mathrm{d}S \qquad \mathbf{F}_\text{body} = \mathbf{F}_\mathrm{G} = \rho_\mathrm{p}\mathcal{V}_\mathrm{p}\mathbf{g}$$

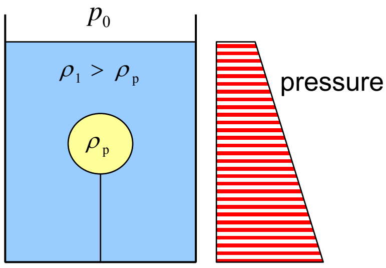
$\mathcal{A}_\mathrm{P}$ = surface area of particle

Newtonian continuous phase: $\mathbb{T}_1 = 2\mu_1\mathbb{D}_1, \quad \mathbb{D}_1 \equiv \frac{1}{2}\left(\nabla\mathbf{v}_1 + (\nabla\mathbf{v}_1)^\mathrm{T}\right)$

$$\Rightarrow \quad \rho_\mathrm{p}\mathcal{V}_\mathrm{p}\frac{\mathrm{d}\mathbf{V}_\mathrm{p}}{\mathrm{d}t} = \rho_\mathrm{p}\mathcal{V}_\mathrm{p}\mathbf{g} + \oiint_{\mathcal{A}_\mathrm{P}}\left(-p_1\mathbb{I} + 2\mu_1\mathbb{D}_1\right)\cdot\hat{\mathbf{n}}_1\mathrm{d}S$$

Special case: hydrostatic situation

- Instructive example:
  - Tank filled with water
  - Ping-pong ball is held under water by a thread
  - Ping-pong ball and water are at rest



$$p_1 = p_{1,\text{hydrostatic}} = p_0 + \rho_1 \mathbf{g}\cdot\mathbf{x}$$
$$\mathbb{T}_1 = \mathbb{O}$$

$$\mathbf{F}_{\text{surface}} = \oiint_{\mathcal{A}_P} \left(-p_1 \mathbb{I} + \mathbb{T}_1\right)\cdot \hat{\mathbf{n}}_1 \,\mathrm{d}S$$

$$\Rightarrow \mathbf{F}_{\text{surface}} = -\oiint_{\mathcal{A}_P} \left(p_0 + \rho_1 \mathbf{g}\cdot\mathbf{x}\right)\hat{\mathbf{n}}_1 \,\mathrm{d}S = -\iiint_{\mathcal{V}_p} \rho_1 \mathbf{g}\,\mathrm{d}V = \boxed{\underbrace{-\mathcal{V}_p \rho_1 \mathbf{g}}_{\text{buoyancy force}}}$$

Archimedes principle

The resulting force on the particle surface

- Splitting of the pressure in two contributions
  - hydrostatic part due to gravity
  - hydrodynamic part

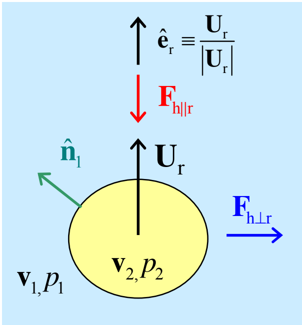
$$p_1 = \rho_1 \mathbf{g}\cdot\mathbf{x} + p_{1,\text{dyn}} \Rightarrow \mathbf{F}_{\text{surface}} = \underbrace{-\mathcal{V}_p \rho_1 \mathbf{g}}_{\text{buoyancy force}} + \underbrace{\oiint_{\mathcal{A}_p} \left(-p_{1,\text{dyn}} \mathbb{I} + 2\mu_1 \mathbb{D}_1\right)\cdot \hat{\mathbf{n}}_1 \,\mathrm{d}S}_{\text{hydrodynamic force } \mathbf{F}_{\text{hydr}}}$$

$$\Rightarrow \underbrace{\rho_p \mathcal{V}_p \frac{\mathrm{d}\mathbf{V}_p}{\mathrm{d}t}}_{\text{inertia force}} = \underbrace{\left(\rho_p - \rho_1\right)\mathcal{V}_p \mathbf{g}}_{\mathbf{F}_{\text{grav}} + \mathbf{F}_{\text{buoy}}} + \boxed{\underbrace{\oiint_{\mathcal{A}_p} \left(-p_{1,\text{dyn}} \mathbb{I} + 2\mu_1 \mathbb{D}_1\right)\cdot \hat{\mathbf{n}}_1 \,\mathrm{d}S}_{\mathbf{F}_{\text{hydr}}}}$$

<u>Problem:</u> determination of hydrodynamic force

The hydrodynamic force on a particle

- The hydrodynamic force is non-zero only if there is a relative motion between particle and surrounding fluid, $\mathbf{U}_\mathrm{r} \equiv \mathbf{V}_\mathrm{p} - \mathbf{U}_\mathrm{c}$
  - $\mathbf{V}_\mathrm{p}$ = translational velocity of center-of-mass of particle
  - $\mathbf{U}_\mathrm{c}$ = characteristic velocity of continuous phase (problem dependent)
- Split of the hydrodynamic force
  - component $\mathbf{F}_{\mathrm{h}\|\mathrm{r}}$ acts opposite to $\hat{\mathbf{e}}_\mathrm{r}$
  - component $\mathbf{F}_{\mathrm{h}\perp\mathrm{r}}$ acts normal to $\hat{\mathbf{e}}_\mathrm{r}$



$$\mathbf{F}_\mathrm{hydr} = \oiint_{\mathcal{A}_\mathrm{p}} \left(-p_{1,\mathrm{dyn}}\mathbb{I} + 2\mu_1\mathbb{D}_1\right)\cdot\hat{\mathbf{n}}_1\,\mathrm{d}S$$
$$= \underbrace{\left(\mathbf{F}_\mathrm{hydr}\cdot\hat{\mathbf{e}}_\mathrm{r}\right)\left(-\hat{\mathbf{e}}_\mathrm{r}\right)}_{\mathbf{F}_{\mathrm{h}\|\mathrm{r}}} + \underbrace{\left[\mathbf{F}_\mathrm{hydr} - \left(\mathbf{F}_\mathrm{hydr}\cdot\hat{\mathbf{e}}_\mathrm{r}\right)\left(-\hat{\mathbf{e}}_\mathrm{r}\right)\right]}_{\mathbf{F}_{\mathrm{h}\perp\mathrm{r}}}$$

The hydrodynamic force on a rigid sphere

- Rigid sphere of diameter d_p moves with velocity $\mathbf{V}_\mathrm{p} = V_\mathrm{p}\hat{\mathbf{e}}_\mathrm{r}$ in creeping flow through an otherwise stagnant fluid
  $\Rightarrow$ characteristic velocity $\mathbf{U}_\mathrm{c} = 0$ so that $\mathbf{U}_\mathrm{r} = \mathbf{V}_\mathrm{p}$

$$\mathbf{F}_\mathrm{hydr} = \underbrace{-3\pi\mu_1 d_\mathrm{p} V_\mathrm{p}\hat{\mathbf{e}}_\mathrm{r}}_{\text{Stokes drag force}} \underbrace{-\frac{1}{2}\mathcal{V}_\mathrm{p}\rho_1\frac{\mathrm{d}V_\mathrm{p}}{\mathrm{d}t}\hat{\mathbf{e}}_\mathrm{r}}_{\text{Added mass force}} \underbrace{-\frac{3}{2}\sqrt{\pi\mu_1\rho_1}\,d_\mathrm{p}^2\hat{\mathbf{e}}_\mathrm{r}\int_0^t \frac{\mathrm{d}V_\mathrm{p}(\tau)/\mathrm{d}\tau}{\sqrt{t-\tau}}\mathrm{d}\tau}_{\text{Basset history force}}$$

Sir George Gabriel Stokes 1819-1903

- The transversal force component is zero
- Drag and Basset force are due to fluid viscosity (μ_1)
- Added mass is due to fluid inertia (ρ_1)

The hydrodynamic force on a rigid sphere

$$\mathbf{F}_{\text{hydr}} = \underbrace{-3\pi\mu_1 d_\text{p} V_\text{p} \hat{\mathbf{e}}_\text{r}}_{\text{Stokes drag force}} \underbrace{-\frac{1}{2}\mathcal{V}_\text{p}\rho_1 \frac{\mathrm{d}V_\text{p}}{\mathrm{d}t}\hat{\mathbf{e}}_\text{r}}_{\text{Added mass force}} \underbrace{-\frac{3}{2}\sqrt{\pi\mu_1\rho_1}\, d_\text{p}^2 \hat{\mathbf{e}}_\text{r} \int_0^t \frac{\mathrm{d}V_\text{p}(\tau)/\mathrm{d}\tau}{\sqrt{t-\tau}}\mathrm{d}\tau}_{\text{Basset history force}}$$

- Stokes drag depends on instantaneous particle velocity
- Added mass force depends on instantaneous particle acceleration
- Basset force depends on history of particle acceleration

- **Generalization for the hydrodynamic force:**

$$\mathbf{F}_{\text{hydr}} = \mathbf{F}_{\text{drag}} + \mathbf{F}_{\text{am}} + \mathbf{F}_{\text{hist}} + \mathbf{F}_{\text{lift}}$$

In the general case these forces must be determined by experiments

The two-fluid model *Repetition*

Set of equations of the two-fluid model:

$$\frac{\partial \alpha_1\rho_1 \overline{\mathbf{v}_1}^{V_1}}{\partial t} + \nabla\cdot\alpha_1\rho_1 \overline{\mathbf{v}_1}^{V_1}\overline{\mathbf{v}_1}^{V_1} = -\nabla\alpha_1 p + \nabla\cdot\alpha_1\mu_1\left(\nabla\overline{\mathbf{v}_1}^{V_1} + \left(\nabla\overline{\mathbf{v}_1}^{V_1}\right)^\text{T}\right) + \alpha_1\rho_1\mathbf{g} + \mathbf{M}_1$$

$$\frac{\partial \alpha_2\rho_2 \overline{\mathbf{v}_2}^{V_2}}{\partial t} + \nabla\cdot\alpha_2\rho_2 \overline{\mathbf{v}_2}^{V_2}\overline{\mathbf{v}_2}^{V_2} = -\nabla\alpha_2 p + \nabla\cdot\alpha_2\mu_2\left(\nabla\overline{\mathbf{v}_2}^{V_2} + \left(\nabla\overline{\mathbf{v}_2}^{V_2}\right)^\text{T}\right) + \alpha_2\rho_2\mathbf{g} + \mathbf{M}_2$$

$$\frac{\partial \alpha_1\rho_1}{\partial t} + \nabla\cdot\alpha_1\rho_1\overline{\mathbf{v}_1}^{V_1} = 0 \qquad \frac{\partial \alpha_2\rho_2}{\partial t} + \nabla\cdot\alpha_2\rho_2\overline{\mathbf{v}_2}^{V_2} = 0 \qquad \mathbf{M}_1 + \mathbf{M}_2 = \frac{1}{V}\iint_{S_1\cap V}\sigma H\hat{\mathbf{n}}_1\mathrm{d}S$$

Closure assumption of the two-fluid model:

Constitutive equation for momentum transfer term $\mathbf{M}_1$

$$\mathbf{M}_1 = -\frac{1}{V}\iint_{S_1\cap V}\left[-p_1\mathbb{I} + \mu_1\left(\nabla\mathbf{v}_1 + (\nabla\mathbf{v}_1)^\text{T}\right)\right]\cdot\hat{\mathbf{n}}_1\mathrm{d}S = \mathbf{M}_1(\rho_1,\rho_2,\mu_1,\mu_2,\sigma,\alpha_1,\overline{\mathbf{v}_1}^{V_1},\overline{\mathbf{v}_2}^{V_2},\ldots)$$

Pressure split for term $\mathbf{M}_k$

$$\mathbf{F}_{\text{surface}} = \oint\!\!\oint_{\mathcal{A}_P} \left(-p_1 \mathbb{I} + 2\mu_1 \mathbb{D}_1\right)\cdot \hat{\mathbf{n}}_1 \mathrm{d}S$$

$$p_1 = \rho_1 \mathbf{g}\cdot\mathbf{x} + p_{1,\text{dyn}}$$

$$\Rightarrow \mathbf{F}_{\text{surface}} = \mathbf{F}_{\text{buoy}} + \mathbf{F}_{\text{hydr}}$$

$$\mathbf{M}_k = -\frac{1}{V}\iint_{S_i \cap V} \left(-p_k \mathbb{I} + 2\mu_k \mathbb{D}_k\right)\cdot \hat{\mathbf{n}}_k \mathrm{d}S$$

$$p_k \equiv \frac{1}{A_i}\iint_{S_i} p_k \mathrm{d}S + p_k' = \overline{p_k}^{S_i} + p_k'$$

$$\Rightarrow \mathbf{M}_k = \overline{p_k}^{S_i} \nabla \alpha_k + \mathbf{M}_{k,\text{h}}$$

"hydrostatic part"

"hydrodynamic part"

Pressure split for term $\mathbf{M}_k$

Introducing this result in the momentum equation for phase k:

$$\frac{\partial \alpha_k \rho_k \overline{\mathbf{v}_k}^{V_k}}{\partial t} + \nabla\cdot\alpha_k \rho_k \overline{\mathbf{v}_k}^{V_k}\,\overline{\mathbf{v}_k}^{V_k} = -\alpha_k \nabla \overline{p_k}^{V_k} - \left(\overline{p_k}^{V_k} - \overline{p_k}^{S_i}\right)\nabla\alpha_k + \nabla\cdot\alpha_k \mathbb{T}_k + \alpha_k \rho_k \mathbf{g} + \mathbf{M}_{k,\text{h}}$$

<u>Assumption:</u> $\overline{p_1}^{V_1} = \overline{p_2}^{V_2} = \overline{p}^{S_i} = p$

<u>Momentum equation for phase k in final form:</u>

$$\frac{\partial \alpha_k \rho_k \overline{\mathbf{v}_k}^{V_k}}{\partial t} + \nabla\cdot\alpha_k \rho_k \overline{\mathbf{v}_k}^{V_k}\,\overline{\mathbf{v}_k}^{V_k} = -\alpha_k \nabla p + \nabla\cdot\alpha_k \mathbb{T}_k + \alpha_k \rho_k \mathbf{g} + \boxed{\mathbf{M}_{k,\text{h}}}$$

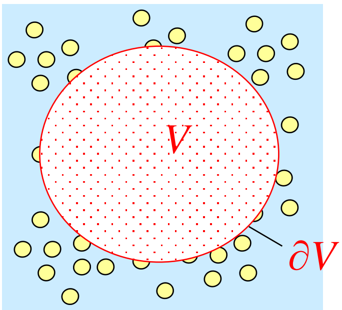
<u>Jump condition:</u> $\mathbf{M}_{1,\text{h}} + \mathbf{M}_{2,\text{h}} = \frac{1}{V}\iint_{S_i \cap V} \sigma H \hat{\mathbf{n}}_1 \mathrm{d}S$

Close set of eqs. by model for $\mathbf{M}_{1,\text{h}}$

The two-fluid model for <u>disperse flow</u>

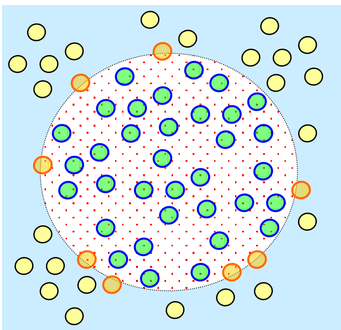
<u>Assumptions:</u>

1. The volume of the individual particles is much smaller than the averaging volume



$$\boxed{\mathcal{V}_{\mathrm{p}} \ll V}$$

The two-fluid model for <u>disperse flow</u>



N_{p} = number of particles that are fully within V and do not cut ∂V

M_{p} = number of particles that cut ∂V

<u>Assumptions:</u>

2. $N_p \gg M_p$

$$\mathbf{M}_{1,\mathrm{h}} = -\frac{1}{V}\iint\limits_{S_1 \cap V} \left(-p_1'\mathbb{I} + 2\mu_1\mathbb{D}_1\right)\cdot\hat{\mathbf{n}}_1 \mathrm{d}s \approx -\frac{1}{V}\sum_{j=1}^{N_{\mathrm{p}}} \oiint\limits_{\mathcal{A}_{\mathrm{p}}^j} \left(-p_{1,\mathrm{dyn}}\mathbb{I} + 2\mu_1\mathbb{D}_1\right)\cdot\hat{\mathbf{n}}_1 \mathrm{d}s = -\frac{1}{V}\sum_{j=1}^{N_{\mathrm{p}}} \mathbf{F}_{\mathrm{hydr}}^j$$

$$\mathbf{M}_{1,\mathrm{h}} + \mathbf{M}_{2,\mathrm{h}} = 0$$

Surface tension force disappears from jump condition!

The two-fluid model for disperse flow

Assumptions:

3. The flow is mono-disperse
   – all particles have the same size (volume $\mathcal{V}_\mathrm{p} = \pi d_\mathrm{eq}^3/6$)
   – all particles experience the same forces

$$\mathbf{M}_{1,\mathrm{h}} \approx -\frac{1}{V}\sum_{j=1}^{N_\mathrm{p}} \mathbf{F}_\mathrm{hydr}^j \approx -\frac{N_\mathrm{p}}{V}\mathbf{F}_\mathrm{hydr} = -n_\mathrm{p}\mathbf{F}_\mathrm{hydr}$$

n_p = local particle number density, i.e. the local number of particles in averaging volume V

$$n_\mathrm{p} = \frac{N_\mathrm{p}}{V} = \frac{N_\mathrm{p}\mathcal{V}_\mathrm{p}}{V}\frac{1}{\mathcal{V}_\mathrm{p}} = \frac{\alpha_2}{\mathcal{V}_\mathrm{p}} = \frac{6\alpha_2}{\pi d_\mathrm{eq}^3} \quad \Rightarrow \quad \mathbf{M}_{1,\mathrm{h}} \approx -\frac{\alpha_2}{\mathcal{V}_\mathrm{p}}\mathbf{F}_\mathrm{hydr} = -\frac{6\alpha_2}{\pi d_\mathrm{eq}^3}\mathbf{F}_\mathrm{hydr}$$

Modeling of the hydrodynamic force

$$\mathbf{F}_\mathrm{hydr} = \mathbf{F}_\mathrm{drag} + \mathbf{F}_\mathrm{am} + \mathbf{F}_\mathrm{hist} + \mathbf{F}_\mathrm{lift}$$

$$\begin{aligned}\mathbf{M}_{1,\mathrm{h}} &= -\frac{\alpha_2}{\mathcal{V}_\mathrm{p}}\mathbf{F}_\mathrm{hydr} = -\frac{\alpha_2}{\mathcal{V}_\mathrm{p}}\left(\mathbf{F}_\mathrm{drag} + \mathbf{F}_\mathrm{vm} + \mathbf{F}_\mathrm{hist} + \mathbf{F}_\mathrm{lift}\right) \\ &= \mathbf{M}_{1,\mathrm{drag}} + \mathbf{M}_{1,\mathrm{vm}} + \mathbf{M}_{1,\mathrm{hist}} + \mathbf{M}_{1,\mathrm{lift}}\end{aligned}$$

Jump conditions: $\mathbf{M}'_{2,\mathrm{drag}} = -\mathbf{M}'_{1,\mathrm{drag}}$ $\quad \mathbf{M}'_{2,\mathrm{vm}} = -\mathbf{M}'_{1,\mathrm{vm}}$

$\mathbf{M}'_{2,\mathrm{hist}} = -\mathbf{M}'_{1,\mathrm{hist}}$ $\quad \mathbf{M}'_{2,\mathrm{lift}} = -\mathbf{M}'_{1,\mathrm{lift}}$

The history force will be neglected: $\mathbf{M}'_{1,\mathrm{hist}} = -\mathbf{M}'_{2,\mathrm{hist}} \approx 0$

Modeling of the drag contribution

$$\mathbf{F}_{\text{drag}} = -\frac{1}{2}\rho_1 A_{\text{pcs}} C_{\text{D}} \mathbf{U}_{\text{r}} \left|\mathbf{U}_{\text{r}}\right|$$

$$\mathbf{U}_{\text{r}} = \overline{\mathbf{v}_2}^{V_2} - \overline{\mathbf{v}_1}^{V_1}$$

$$A_{\text{pcs}} = \frac{\pi}{4} d_{\text{eq}}^2 \qquad \mathcal{V}_{\text{p}} = \frac{\pi}{6} d_{\text{eq}}^3$$

$$\Rightarrow \quad \mathbf{M}_{2,\text{drag}} = -\mathbf{M}_{1,\text{drag}} = -\frac{\alpha_2}{\mathcal{V}_{\text{p}}} \mathbf{F}_{\text{drag}} = -\frac{3}{4} C_{\text{D}} \rho_1 \frac{\alpha_2}{d_{\text{eq}}} \left|\overline{\mathbf{v}_2}^{V_2} - \overline{\mathbf{v}_1}^{V_1}\right| \left(\overline{\mathbf{v}_2}^{V_2} - \overline{\mathbf{v}_1}^{V_1}\right)$$

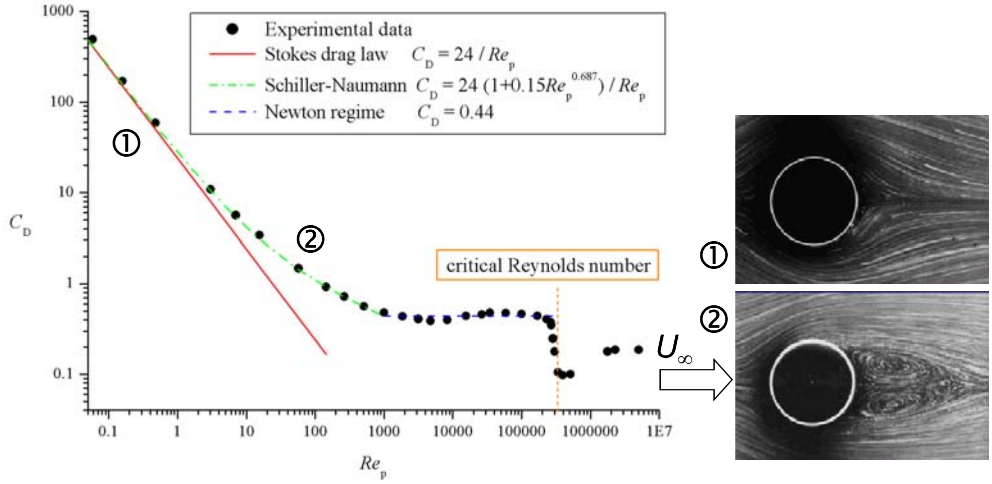
Depends on geometry of particle

Equivalent bubble diameter must be known !

Modeling of the drag force

- Dilute flows (low volume fraction of disperse phase)
  - The interaction between particles can be neglected
  - For C_D drag laws obtained for “isolated” particles can be used
  - Approximate condition: $\alpha_2 < 0.1\%$
- Dense flows (high volume fraction of disperse phase)
  - Because of significant particle-particle interaction the velocity of a particle in a swarm differs from that of an isolated particle
  - Drag laws obtained for isolated particles must be corrected
  - The correction factor depends on α_2

Drag coefficient for a rigid sphere



Drag laws for rigid spheres

Rigid sphere in dilute flow

$$C_D(Re_p) = \begin{cases} \dfrac{24}{Re_p}\left(1 + 0.15 Re_p^{0.687}\right) & \text{for} \quad Re_p < 1000 \\ 0.44 & \text{for} \quad 1000 < Re_p < 3 \times 10^6 \end{cases}$$

$$Re_p = \frac{\rho_1 d_{eq} \left| \overline{\mathbf{v}_2}^{V_2} - \overline{\mathbf{v}_1}^{V_1} \right|}{\mu_1}$$

Correlation of Schiller & Naumann (1933)

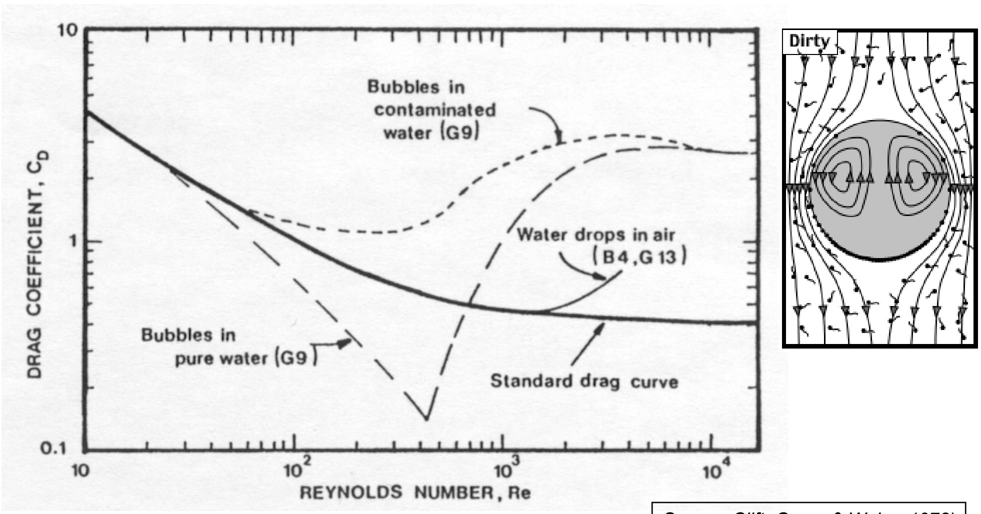
Newton regime

Rigid spheres in dense flow

$$C_D(Re'_p, \alpha_1) = \alpha_1^{-1.65} \max\left\{ \frac{24}{Re'_p}\left(1 + 0.15 Re_p'^{0.687}\right), 0.44 \right\} \quad \text{with} \quad Re'_p = \alpha_1 Re_p$$

Correlation of Wen & Yu valid for $\alpha_2 < 0.2$

Drag coefficient for air bubbles in water



Source: Clift, Grace & Weber 1978)

Bubble drag laws for dilute flow

Model of Tomiyama:

– pure system

$$C_D = \max\left[\min\left\{\frac{16}{Re_p}\left(1+0.15Re_p^{0.687}\right), \frac{48}{Re_p}\right\}, \frac{8}{3}\frac{Eö_B}{Eö_B+4}\right]$$

– slightly contaminated system

$$C_D = \max\left[\min\left\{\frac{24}{Re_p}\left(1+0.15Re_p^{0.687}\right), \frac{72}{Re_p}\right\}, \frac{8}{3}\frac{Eö_B}{Eö_B+4}\right]$$

– strongly contaminated system

$$C_D = \max\left[\frac{24}{Re_p}\left(1+0.15Re_p^{0.687}\right), \frac{8}{3}\frac{Eö_B}{Eö_B+4}\right]$$

Schiller-Naumann for bubble (H-R correction)

Potential flow around ridig sphere

Cap bubble

Schiller-Naumann for rigid sphere

Potential flow around bubble

Modeling of the added mass force

- Added mass force for sphere in creeping flow (analytical result)

$$\boxed{\mathbf{F}_{\mathrm{vm}} = \frac{1}{2}\mathcal{V}_{\mathrm{p}}\rho_1 \frac{\mathrm{d}V_{\mathrm{p}}}{\mathrm{d}t}\hat{\mathbf{e}}_{\mathrm{r}}}$$

- Added mass force in two-fluid model

$$\boxed{\mathbf{M}'_{2,\mathrm{vm}} = -\mathbf{M}'_{1,\mathrm{vm}} = C_{\mathrm{vm}}\alpha_2\rho_1\left(\frac{\mathrm{D}_2\overline{\mathbf{v}_2}^{V_2}}{\mathrm{D}t} - \frac{\mathrm{D}_1\overline{\mathbf{v}_1}^{V_1}}{\mathrm{D}t}\right)} \qquad \boxed{\frac{\mathrm{D}_k}{\mathrm{D}t} \equiv \frac{\partial}{\partial t} + \overline{\mathbf{v}_k}^{V_k}\cdot\nabla}$$

- Coefficient of added mass force
  - Single rigid sphere in liquid of infinite extend $\boxed{C_{\mathrm{vm}} = 1/2}$
  - Influence of volume fraction $\boxed{C_{\mathrm{vm}} = \left(1 + 3.26\alpha_2 + 7.7\alpha_2^2\right)/2}$

Modeling of the lift force

- The lift force typically occurs in shear flows
  - Example: shear due to presence of walls
  - The lift force act normal to the relative velocity
- The lift force in the two-fluid model
  - There exist a number of different models, e.g.

$$\boxed{\mathbf{M}_{2,\mathrm{lift}} = -\mathbf{M}_{1,\mathrm{lift}} = -C_{\mathrm{lift}}\alpha_2\rho_1\left(\overline{\mathbf{v}_2}^{V_2} - \overline{\mathbf{v}_1}^{V_1}\right)\times\nabla\times\overline{\mathbf{v}_1}^{V_1}}$$

  - The coefficient C_{lift} depends on Re_{p} and further parameters
  - For $C_{\mathrm{lift}} > 0$ the lift force acts toward the wall
  - For deformed bubbles C_{lift} can become negative!

Further forces in the two-fluid model

- Wall lubrication force
  - Empirically introduced force
  - Act only close to the wall and away from the wall
  - Balances lift force close the wall
  - Avoids unphysical increase of α_2 at the wall
- Turbulent dispersion force
  - Empirically introduced force
  - Turbulence causes a lateral dispersion of particles
  - This effect is modeled by the turbulent dispersion force
  - Force is proportional to the gradient of α_2

Modeling of heat transfer

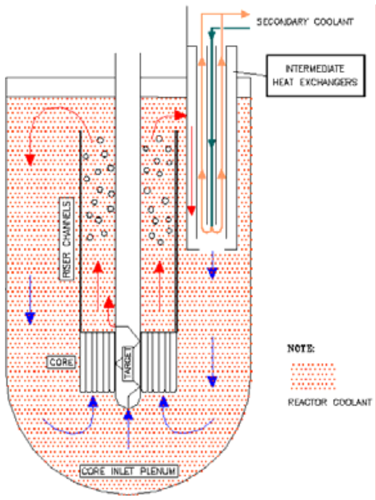
- Equivalent averaging procedures than have been applied to the momentum equation can be used to derive a set of two (interpenetrating) energy equations for the phases
- The energy equations of the phases are coupled by interfacial heat transfer terms which sum up to zero
- The interfacial heat transfer is related to an heat transfer coefficient, which is modeled in terms of an empirical correlation for the Nusselt number
- Ranz and Marshall correlation: $\boxed{Nu_{\mathrm{p}} = 2.0 + 0.6 Re_{\mathrm{p}}^{1/2} Pr^{1/3}}$

Standard two-fluid model for disperse flow

- Main assumptions
  - Particle volume is much smaller than averaging volume
  - Surface tension force is neglected
  - All particles have the same size (mono-disperse flow)
  - The equivalent diameter of the particles must be known
- Modeled forces in order of relevance
  - <u>Drag force</u>, added mass force, lift force, ...
- Disadvantage
  - The model does not account for coalescence or break-up of bubbles or drops which result in a size-distribution

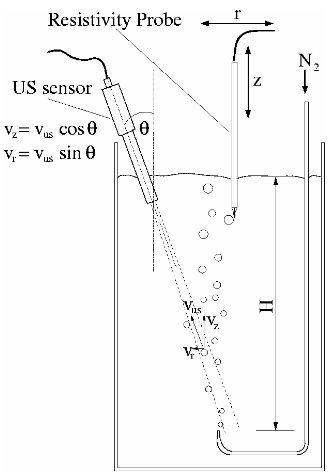
Example for application of two-fluid model

- Results from FP5 project ASCHLIM = Assessment of CFD codes for heavy liquid metals
- To enhance the flow circulation within an ADS the injection of gas bubbles in heavy liquid metal was under consideration
- Question: Can CFD codes predict the rise of gas bubbles in HLM?



Experiments in lead-bismuth (Pb-Bi)

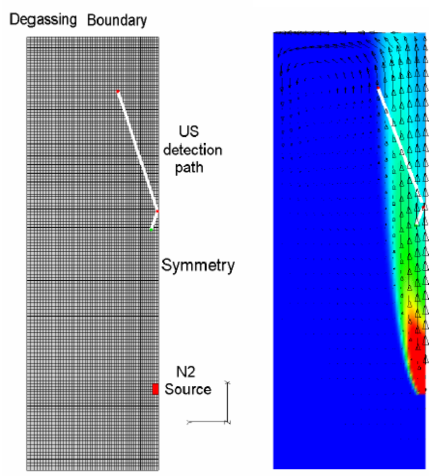
- Cylinder with 125 mm diameter
- Injection depth H = 150 mm
- Temperature Pb-Bi: 170ºC
- Nitrogen bubble with equivalent diameter of 4 – 6 mm
- Measured data
  - local gas content (resistivity probe)
  - Bubble velocity and profile of liquid velocity (Ultra sound sensor)



Source: Forschungszentrum Rossendorf, Germany

Recalculation of lead-bismuth experiments

- Two fluid model calculations
  - Computer code: CFX-4
  - Axisymmetry
  - Structured grid with 142 x 53 mesh cells
  - **Forces (constant bubble diameter)**
    - **Drag force**
    - **Lift force**
    - **Wall lubrication force**
    - **Turbulent dispersion force**
  - For liquid phase use of turbulence model
  - Difference scheme of 2nd order



Source: G. Mercurio, ENEA, Italy

Recalculation of lead-bismuth experiments

Comparison with experiment

Gas velocity

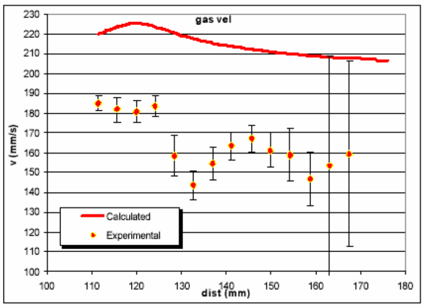


Figure 4.2.1 Calculated and experimental gas velocity along the detection path (Q= 0.034 cm^3/s).

Liquid velocity

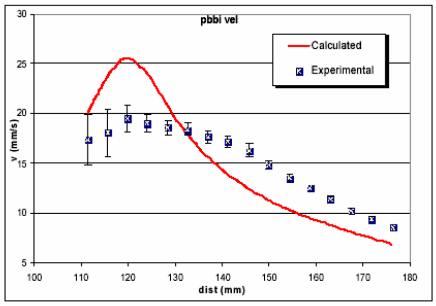


Figure 4.2.2 Calculated and experimental PbBi velocity along the detection path (Q= 0.034 cm^3/s).

Source: G. Mercurio, ENEA, Italy

Recalculation of lead-bismuth experiments

- Results of the two-fluid model
  - Use of standard drag laws results in bad agreement with experiments
  - Better agreement possible by tuning model coefficients
- Problematic of gas bubbles in liquid metals
  - Very low value of the Morton number $M \approx 10^{-13}$
  - **No experimental correlations available for** C_D
  - Bubbles significantly expand as they rise
  - Do coalescence and break-up play a role?
  - Can the turbulence model developed for single phase flow be used for bubbly flow?

Parameters in experiment

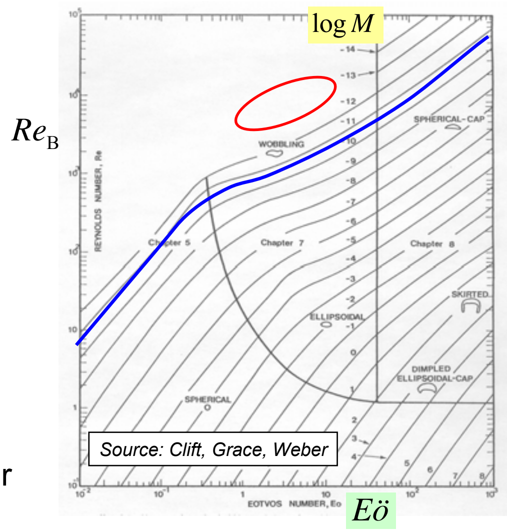
- Morton number

$$M = \frac{g \Delta \rho \mu_c^4}{\rho_c^2 \sigma^3} \approx 10^{-13}$$

- Eötvös number

$$Eö = \frac{g \Delta \rho d_{\mathrm{eq}}^2}{\sigma} \approx 4 - 10$$

- Bubble shape is not known (shape is probably unstable)
- Blue line: air bubbles in water



Summary standard two-fluid model

- The standard two-fluid model is the “working horse” for the computation of technical two-phase flows
- Detailed discussion of the standard two-fluid model for disperse flow
- The two-fluid model can be used for any flow regime
  - Stratified flow, annular flow, slug flow, ...
  - But: the modeling of $\mathbf{M}_{1h}$ must take into account the flow regime (the flow regime must be known a priori!)
  - The standard two-fluid model can not be used to compute the transition from one flow regime to another flow regime

Extensions of the standard two-fluid model

- Population balance modeling
  - Represent the disperse phase by certain “classes”
- Transport eq. for specific interfacial area concentration
  - Introduction of a „local“ bubble diameter
- Four field two-fluid model
  - Extension of the two-fluid model to two fields per phase / fluid
  - Each phase can exist as continuous and disperse

Population balance for bubble classes

- Dispersed flows often show a wide range of particle diameters
- Basic idea of population balance model:
  - Bubbles are classified in classes
  - For each class a separate mass and momentum equation is solved
  - One field for continuous phase + N fields for disperse phase
    - Each field $j = 1,...,N$ represents particles with a certain diameter or diameter range
    - Special case $N = 1$: standard two-fluid model
- Problem
  - Modeling of source and sink terms in mass balance equations for the individual populations (coalescence, break-up)
  - Depending on N the method can require very large CPU times

Organization of Lecture

- Fundamental equations for multi-fluid flows
- Continuous field models
  - Homogenous model
  - Algebraic slip model
  - Two-fluid model
- **Euler-Lagrange method**
- Interface resolving simulation methods

Basic idea of Euler-Lagrange model

- Euler approach for continuous phase (carrier phase)
- Lagrange approach for disperse phase
  - equation of motion is solved for individual particles
  - this is done for a large number of particles or particle clusters
  - representative disperse phase quantities are obtained from ensemble averaging
- Model can be used only for disperse flow (ideally suited for rigid particles)
- Particles are considered as point-particle and the flow around a particle is not resolved

Equation of motion for the particle

For constant particle mass m_p the equation of motion reads:

$$\underbrace{\rho_\mathrm{p}\mathcal{V}_\mathrm{p}}_{m_\mathrm{p}}\frac{\mathrm{d}\mathbf{V}_\mathrm{p}}{\mathrm{d}t} = \rho_\mathrm{p}\mathcal{V}_\mathrm{p}\mathbf{g} + \mathbf{F}_\mathrm{surface}$$

$$\mathbf{F}_\mathrm{surface} = \underbrace{-\mathcal{V}_\mathrm{p}\rho_\mathrm{l}\mathbf{g}}_{\text{buoyancy force}} + \underbrace{\left(-\mathcal{V}_\mathrm{p}P_\mathrm{pd}\hat{\mathbf{e}}_\mathrm{pd}\right)}_{\substack{\text{body force due to}\\ \text{external pressure drop}}} + \underbrace{\oiint_{\mathcal{A}_\mathrm{p}}\left(-p_{\mathrm{l,dyn}}\mathbb{I} + 2\mu_\mathrm{l}\mathbb{D}_\mathrm{l}\right)\cdot\hat{\mathbf{n}}_\mathrm{l}\,\mathrm{d}S}_{\text{hydrodynamic force } \mathbf{F}_\mathrm{hydr}}$$

$$\mathbf{F}_\mathrm{hydr} = \mathbf{F}_\mathrm{drag} + \mathbf{F}_\mathrm{vm} + \mathbf{F}_\mathrm{hist} + \mathbf{F}_\mathrm{lift}$$

(Pressure is split in 3 contributions:

- *Hydrostatic part due to gravity*
- *Part due to linear external pressure drop*
- *Hydrodynamic part)*

Equation of motion for the particle

$$\rho_\mathrm{p}\mathcal{V}_\mathrm{p}\frac{\mathrm{d}\mathbf{V}_\mathrm{p}}{\mathrm{d}t} = \mathbf{F}_\mathrm{G} + \mathbf{F}_\mathrm{B} + \mathbf{F}_\mathrm{PG} + \mathbf{F}_\mathrm{drag} + \mathbf{F}_\mathrm{vm} + \mathbf{F}_\mathrm{hist} + \mathbf{F}_\mathrm{lift}$$

$\mathbf{F}_\mathrm{G}$ = gravity force

$\mathbf{F}_\mathrm{B}$ = buoyancy force

$\mathbf{F}_\mathrm{PG}$ = Pressure gradient force

$\mathbf{F}_\mathrm{drag}$ = drag force

$\mathbf{F}_\mathrm{am}$ = added mass force

$\mathbf{F}_\mathrm{hist}$ = history force

$\mathbf{F}_\mathrm{lift}$ = transversal lift force

Forces to be modeled

$$\mathbf{V}_\mathrm{p}(t) = \frac{\mathrm{d}\mathbf{X}_\mathrm{p}(t)}{\mathrm{d}t}$$

$\mathbf{X}_\mathrm{p}(t)$ = position of center-of-mass of particle

Modeling of the hydrodynamic forces

$$\mathbf{F}_{\mathrm{drag}} = \frac{1}{2} C_{\mathrm{D}} \rho_{\mathrm{c}} A_{\mathrm{pcs}} \left(\mathbf{U}_{\mathrm{c}} - \mathbf{V}_{\mathrm{p}}\right)\left|\mathbf{U}_{\mathrm{c}} - \mathbf{V}_{\mathrm{p}}\right|$$

$$A_{\mathrm{pcs}} = \frac{\pi}{4} d_{\mathrm{eq}}^2$$

$$\mathbf{F}_{\mathrm{am}} = C_{\mathrm{am}} \rho_{\mathrm{c}} \mathcal{V}_{\mathrm{p}} \frac{\mathrm{d}\left(\mathbf{U}_{\mathrm{c}} - \mathbf{V}_{\mathrm{p}}\right)}{\mathrm{d}t}$$

Here no models for history and lift force:

$$\mathbf{F}_{\mathrm{hist}} \approx 0 \qquad \mathbf{F}_{\mathrm{lift}} \approx 0$$

Characteristic velocity of continuous phase:

$$\mathbf{U}_{\mathrm{c}} = \mathbf{v}_{\mathrm{c}}(\mathbf{x} = \mathbf{X}_{\mathrm{p}})$$

Particle response time

- Consider a particle on which only inertia and drag force act:

$$\rho_{\mathrm{p}} \mathcal{V}_{\mathrm{p}} \frac{\mathrm{d}\mathbf{V}_{\mathrm{p}}}{\mathrm{d}t} = \mathbf{F}_{\mathrm{drag}} = \frac{1}{2} C_{\mathrm{D}} \rho_{\mathrm{c}} A_{\mathrm{pq}} \left(\mathbf{v}_{\mathrm{c}} - \mathbf{V}_{\mathrm{p}}\right)\left|\mathbf{v}_{\mathrm{c}} - \mathbf{V}_{\mathrm{p}}\right|$$

$$A_{\mathrm{pq}} = \frac{\pi}{4} d_{\mathrm{eq}}^2$$

$$\Rightarrow \frac{\mathrm{d}\mathbf{V}_{\mathrm{p}}}{\mathrm{d}t} = \frac{3}{4} \frac{\mu_{\mathrm{c}}}{\rho_{\mathrm{p}} d_{\mathrm{eq}}^2} C_{\mathrm{D}} Re_{\mathrm{p}} \left(\mathbf{v}_{\mathrm{c}} - \mathbf{V}_{\mathrm{p}}\right)$$

Factor has the dimension of a frequency [s^{-1}]

Definition of particle response time:

$$\tau_{\mathrm{p}} \equiv \frac{4}{3} \frac{\rho_{\mathrm{p}} d_{\mathrm{eq}}^2}{\mu_{\mathrm{c}}} \frac{1}{C_{\mathrm{D}} Re_{\mathrm{p}}}$$

Then, the equation of motion becomes:

$$\frac{\mathrm{d}\mathbf{V}_{\mathrm{p}}}{\mathrm{d}t} = \frac{\mathbf{v}_{\mathrm{c}} - \mathbf{V}_{\mathrm{p}}}{\tau_{\mathrm{p}}}$$

Interpretation of particle response time

- Example:
  - Rectilinear motion (one-dimensional case)
  - Constant velocity of continuous phase $v_c = U_\infty = \text{const.}$
  - Particle accelerates from rest
- Equation of motion: $\dfrac{dV_p}{dt} = \dfrac{U_\infty - V_p}{\tau_p}$ where $V_p(0) = 0$
- Solution: $V_p(t) = U_\infty\left(1 - e^{-t/\tau_p}\right)$ $\Rightarrow$ $\dfrac{V_p(\tau_p)}{U_\infty} = 1 - \dfrac{1}{e} \approx 0{,}632$
- The particle response time is the time the particle needs by acceleration to reach 63.2% of its terminal velocity

Particle response time for Stokes flow

Particle response time:

$$\tau_p \equiv \frac{4}{3}\frac{\rho_p d_{eq}^2}{\mu_c}\frac{1}{C_D Re_p} = \frac{\rho_p d_{eq}^2}{18\mu_c}\frac{24}{C_D Re_p}$$

Stokes drag law: $C_D = \dfrac{24}{Re_p}$ $\Rightarrow$ $\dfrac{24}{C_D Re_p} = 1$

The particle response time becomes: $\tau_p = \dfrac{\rho_p d_p^2}{18\mu_c}$

For a 300 µm water droplet in air τ_p is about 30 ms

Time scales for continuous phase

- Characteristic time scale of macroscopic motion

$$\tau_{\mathrm{c,makro}} = \frac{L}{U} = \frac{\text{characteristic macroscopic length}}{\text{characteristic macroscopic velocity}}$$

- Time scale of turbulent velocity fluctuations

$$\tau_{\mathrm{c,turb}} = \frac{k}{\varepsilon} = \frac{\text{kinetic energy of turbulence}}{\text{dissipation rate of } k}$$

- Kolmogorov time scale (time scale of smallest eddies)

$$\tau_{\mathrm{c,K}} \equiv \sqrt{\frac{\nu_{\mathrm{c}}}{\varepsilon}} = \sqrt{\frac{\mu_{\mathrm{c}}}{\rho_{\mathrm{c}}\varepsilon}}$$

Definition of Stokes number

$$St \equiv \frac{\tau_{\mathrm{p}}}{\tau_{\mathrm{c}}} = \frac{\text{particle response time}}{\text{time scale of continuous phase}}$$

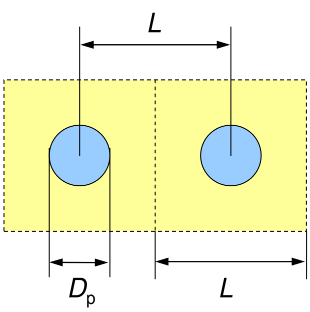
$$St_{\mathrm{makro}} \equiv \frac{\tau_{\mathrm{p}}}{\tau_{\mathrm{c,makro}}} \qquad St_{\mathrm{turb}} \equiv \frac{\tau_{\mathrm{p}}}{\tau_{\mathrm{c,turb}}} \qquad St_{\mathrm{K}} \equiv \frac{\tau_{\mathrm{p}}}{\tau_{\mathrm{c,K}}}$$

- Limiting cases
  - $St_{\mathrm{K}} \rightarrow 0$: The particle completely follows the fluid motion (is approximately true for very small particles)
  - $St_{\mathrm{K}} \rightarrow \infty$: The motion of the particle and that of the continuous phase are totally uncorrelated
  - In praxis both limiting cases hardly occur and the particle responses with time lag to a change of the fluid velocity

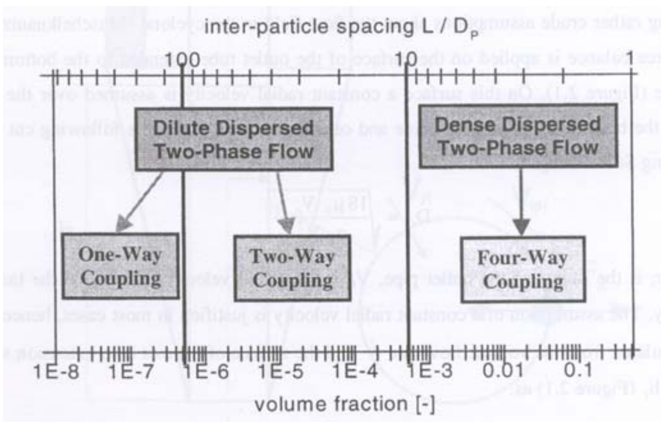
Concepts for interaction of the phases

- One-way coupling
  - The continuous phase influences the particle motion
  - The particles are without influence on the carrier phase
  - No interaction between individual particles
- Two-way coupling
  - Carrier phase and disperse phase influence each other
  - No interaction between individual particles
- Four-way coupling
  - Carrier phase and disperse phase influence each other
  - The interaction between particles is also considered as well as their consequences on the carrier phase

Inter-particle spacing



$$\frac{L}{D_p} = \left(\frac{\pi}{6\alpha_d} \right)^{1/3}$$



Source: S. Elgobashi

One-way coupling

- Particles are without influence on the carrier phase
- The continuous phase flow field can be determined from a single-phase computation
- The steady flow field (laminar flow) or the time averaged flow field (turbulent flow) needs to be computed once only
- Before the Lagrange part is performed the carrier phase flow field $\mathbf{v}_c(\mathbf{x})$ is already known

One-way coupling

- Because there is no interaction between individual particles the particle trajectories can be computed independently

$$\frac{\mathrm{d}\mathbf{V}_{\mathrm{p},j}}{\mathrm{d}t} \approx \frac{\mathbf{V}^{\mathrm{n+1}}_{\mathrm{p},j} - \mathbf{V}^{\mathrm{n}}_{\mathrm{p},j}}{\Delta t} = \frac{\mathbf{F}^n_{\mathrm{G},j} + \mathbf{F}^n_{\mathrm{A},j} + \mathbf{F}^n_{\mathrm{P},j} + \mathbf{F}^n_{\mathrm{drag},j} + \mathbf{F}^n_{\mathrm{vm},j} + \mathbf{F}^n_{\mathrm{hist},j} + \mathbf{F}^n_{\mathrm{lift},j}}{\rho_{\mathrm{p},j}\mathcal{V}_{\mathrm{p},j}}$$

$$\frac{\mathrm{d}\mathbf{X}_{\mathrm{p}}(t)}{\mathrm{d}t} \approx \frac{\mathbf{X}^{n+1}_{\mathrm{p},j} - \mathbf{X}^{n}_{\mathrm{p},j}}{\Delta t} = \mathbf{V}^n_{\mathrm{p},j}$$

- Sequential computation of all particle trajectories on one processor or parallel computation on several processors
- Size and initial position of particles must be varied to well represent the respective probability distribution

One-way coupling

- Local properties of disperse phase such as volume fraction and velocity field are obtained by ensemble averaging over all realizations $j = 1, N_{\mathrm{p}}$
- The number N_{p} of particles tracked is not arbitrary, but must be large enough to well represent the particle population
- This can be tested by performing simulations with different numbers of particles and by comparing the results (Typically 10.000 – 100.000 particles are tracked)

One-way coupling: sequence of computational steps

1.) Generate $d_{\mathrm{p},j}$, $\mathbf{X}^0_{\mathrm{p},j}$ and $\mathbf{V}^0_{\mathrm{p},j}$ as initial condition $(n=0)$

2.) Compute fluid velocity at position $\mathbf{v}_{\mathrm{c}}(\mathbf{x} = \mathbf{X}^n_{\mathrm{p},j})$ by interpolation

3.) Compute $\mathbf{F}^n_{\mathrm{G},j} + \mathbf{F}^n_{\mathrm{B},j} + \mathbf{F}^n_{\mathrm{PG},j} + \mathbf{F}^n_{\mathrm{drag},j} + \mathbf{F}^n_{\mathrm{am},j} + \mathbf{F}^n_{\mathrm{hist},j} + \mathbf{F}^n_{\mathrm{lift},j}$

4.) Compute $\mathbf{V}^{\mathrm{n}+1}_{\mathrm{p},j} = \mathbf{V}^{\mathrm{n}}_{\mathrm{p},j} + \dfrac{\Delta t}{\rho_{\mathrm{p},j}\mathcal{V}_{\mathrm{p},j}}\left(\mathbf{F}^n_{\mathrm{G},j} + \mathbf{F}^n_{\mathrm{B},j} + \mathbf{F}^n_{\mathrm{PG},j} + \mathbf{F}^n_{\mathrm{drag},j} + \mathbf{F}^n_{\mathrm{vm},j} + \mathbf{F}^n_{\mathrm{lift},j}\right)$

5.) Compute $\mathbf{X}^{n+1}_{\mathrm{p},j} = \mathbf{X}^n_{\mathrm{p},j} + \Delta t \mathbf{V}^n_{\mathrm{p},j}$

6.) Set $n = n+1$ and go to step 2; repeate steps 2 - 6 until the particle leaves the computational domain

7.) Go to step 1 and track the next particle $(j = j+1)$

Accounting for turbulence

- In an experiment within a turbulent flow identical particles nominally released at the same position will follow a different path due to local turbulent velocity fluctuations (turbulent dispersion of particles)
- In a computation only the time averaged mean velocity field of the carrier phase is computed
- In the Lagrange step therefore the particle is transported by the mean velocity field and for identical initial conditions each particle follows the same deterministic path (thus there is no turbulent dispersion)

Accounting for turbulence

- Problem: in reality the particle is transported by the local turbulent velocity field and not by the time averaged mean
- Remedy: introduction of a fluctuation velocity $\mathbf{v}_c'$

$$\boxed{\mathbf{v}_c(\mathbf{x},t) = \overline{\mathbf{v}_c}^t(\mathbf{x}) + \mathbf{v}_c'(\mathbf{x},t)}$$

"*random walk*"

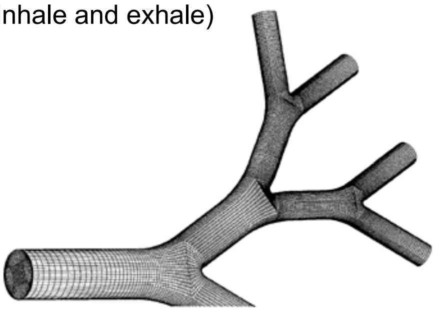
  - Modeling of fluctuation velocity as stochastic process
  - The fluctuations are assumed to obey a Gaussian probability distribution
  - The mean value of the Gaussian is zero
  - The variance of the Gaussian is set to: $\sigma = \sqrt{2k/3}$ (k = turbulent kinetic energy)

Example: particle transport in the human lung

- The lung consists of a network with about 23 branches
  - diameter from 18 mm (trachea) to 0.4 mm
- Questions:
  - where do rigid particles (dust, smoke) deposit
  - how far penetrate drugs in form of sprays
- Euler-Lagrange computations of Zhang et al.

Particle transport in the human lung

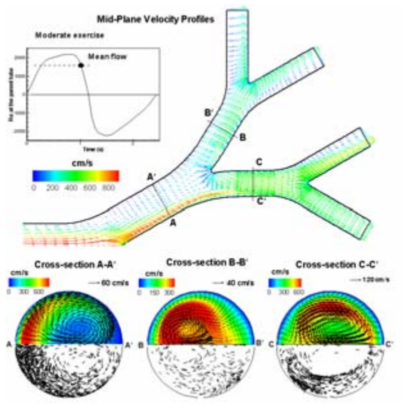
- Computer code CFX-4 extended by user subroutines
- Euler part
  - 3D computations (Finite Volumes) with 360.000 mesh cells
  - Laminar time-dependent gas flow (inhale and exhale)
  - One-way coupling
- Lagrange part
  - only inertia and drag force
  - Particle diameter 3-7 μm
  - $Re_p < 1$, $St_{makro} < 0{,}3$
  - 25000 particles



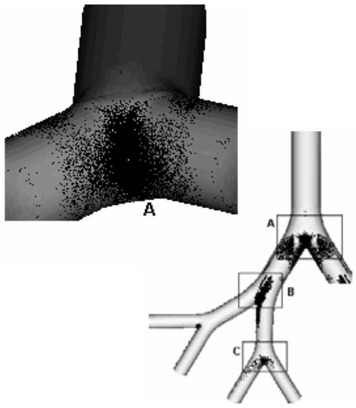
Source: Zhang, Kleinstreuer, Kim, Int. J. Multiphase Flow 28 (2002) 1021-1046

Particle transport in the human lung

Air flow



Particle deposition



Source: Zhang, Kleinstreuer, Kim, Int. J. Multiphase Flow 28 (2002) 1021-1046

Two-way coupling

- The particles act back on the carrier phase
- The carrier phase flow must be computed iteratively or time-dependent
- The time step width of the Lagrange part is usually smaller than that of the Euler part
- The reaction of the particle on the carrier phase in a mesh cell is obtained by considering all particle trajectories that pass this mesh cell within the Eulerian time step
- The phase coupling may result in convergence problems

Four-way coupling: particle collisions

- Two different concepts in literature
  - Direct modeling
  - Statistical modeling based on the kinetic gas theory
- Direct modeling
  - All particles are tracked simultaneously
  - If a collisions between any pair of particles occurs within a time step can be estimated from the particles positions and their relative velocity
  - If a collision occurs then the translatory and angular velocity of the particles are modified from the conservation equations for linear and angular momentum taking into account Coulomb friction
  - Disadvantage: high requirements for CPU time and main memory

Four-way coupling: particle collisions

- Statistical modeling of particle collisions
  - The particle trajectories are computed independently
  - There is no information available about neighboring particles
  - Based on the kinetic gas theory a collision probability is computed
  - Fictitious collision partners are generated based on local probability density functions for particle diameter and velocity
- Development of models for two- and four-way coupling is an actual field of research

Organization of Lecture

- Fundamental equations for multi-fluid flows
- Continuous field models
  - Homogenous model
  - Algebraic slip model
  - Two-fluid model
- Euler-Lagrange method
- **Interface resolving simulation methods**

Weaknesses of models discussed up to now

- Euler-Lagrange model
  - Suitable for disperse flows with low void fraction (< 10%)
  - Difficulty to account for interaction of disperse elements and for feedback on continuous phase
- Homogeneous model and algebraic slip model
  - Only suitable for very special flow situations
    (HM: gravity dominated stratified flows, ASM: well defined disperse flows)
- Euler-Euler model (two fluid model)
  - The exchange terms between the phases which must be modeled do strongly depend on the flow regime
  - Therefore the flow regime is assumed to be known a priori
  - Surface tension force is not considered explicitly, though it has a significant influence on flow regime and shape of bubbles and drops

Idea of interface resolving simulation methods

- The basic multi-fluid flow equations are solved „directly"
  - Directly means (almost) without empirical models ("DNS")
  - The simulation is in general 3D and time-dependent
  - High spatial and temporal resolution (Δx and Δt are very small)
- Advantages:
  - Surface tension force is explicitly accounted for
  - Phase distributions and shape of bubbles/drops is simulation result
  - Full 3D time-resolved information about all flow quantities
- Disadvantages:
  - Very high computational cost as compared to TFM and ELM
  - Mainly suitable for basic research, not for general engineering practice

Problematic issues

- Physics
  - The phases are separated by the interface
  - The interface moves and deforms
  - Density, viscosity and pressure are discontinuous at the interface
- Numerical representation
  - No phase change $\Rightarrow$ phase distribution is described by

$$\boxed{\frac{\mathrm{D}X_k}{\mathrm{D}t} = \frac{\partial X_k}{\partial t} + \mathbf{v}_k \cdot \nabla X_k = 0}$$

  - Discretization with finite differences results in unphysical "smearing" of the interface because of numerical diffusion
  - Special numerical methods required to describe phase distribution

Description of phase distribution

- Three different methods are commonly in use
  - Volume-of-Fluid method (originally developed by Hirt&Nicols)
  - Level-set method (originally developed by Osher)
  - Front tracking method (originally developed by Tryggvason)
- Common features of all methods
  - Mainly for incompressible (or weakly compressible) phases
  - Based on single-field momentum equation (similar to HM and ASM)
  - Assumption: grid size is so small that in mesh cells containing both phases the relative velocity between the phases can be neglected (locally homogeneous model)

Equations of the Volume-of-Fluid method

- Assumption: averaging volume V = volume of a mesh cell
- Notation:

$$\alpha_1 = f \equiv \frac{1}{V}\iiint_V X_1 \mathrm{d}V \quad \Rightarrow \quad \alpha_2 = 1 - f$$

$$\mu_\mathrm{m} \equiv f\mu_1 + (1-f)\mu_2 \qquad \rho_\mathrm{m} \equiv f\rho_1 + (1-f)\rho_2 \qquad \mathbf{v}_\mathrm{m} \equiv \frac{f\rho_1 \overline{\mathbf{v}_1}^{V_1} + (1-f)\rho_2 \overline{\mathbf{v}_2}^{V_2}}{f\rho_1 + (1-f)\rho_2}$$

$$\frac{\partial f}{\partial t} + \nabla \cdot f\mathbf{v}_\mathrm{m} = 0 \qquad \nabla \cdot \mathbf{v}_\mathrm{m} = 0$$

$$\frac{\partial \rho_\mathrm{m}\mathbf{v}_\mathrm{m}}{\partial t} + \nabla \cdot \rho_\mathrm{m}\mathbf{v}_\mathrm{m}\mathbf{v}_\mathrm{m} = -\nabla p_\mathrm{m} + \rho_\mathrm{m}\mathbf{g} + \nabla \cdot \mu_\mathrm{m}\left(\nabla \mathbf{v}_\mathrm{m} + (\nabla \mathbf{v}_\mathrm{m})^\mathrm{T}\right) + \frac{1}{V}\iint_{S_\mathrm{i}\cap V} \sigma\kappa\hat{\mathbf{n}}_1 \mathrm{d}S$$

Concept for solution of f – equation

- Because the interface is well resolved the liquid volume fraction f has large gradients
- To avoid numerical smearing of the interface the f - equation is not solved by a difference schemes but in a rather “geometrical” manner
- Representation of f – equation in integral form
  - Derivation from continuity equation for phase 1
- Solution proceeds in two steps
  - Reconstruction of interface
  - Advection of interface and computation of volume fluxes of phase 1 across the faces of the mesh cell

Derivation of f – equation in integral form

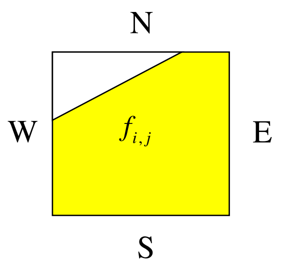
- Continuity equation for phase 1

$$\boxed{\frac{\partial \rho_1}{\partial t} + \nabla \cdot \rho_1 \mathbf{v}_1 = 0}$$

- Multiplication with X_1, integration over mesh volume V, division by ρ_1=const. and use of Gauß divergence theorem yields

$$\boxed{\frac{\partial f}{\partial t} + \frac{1}{V} \oiint_{\partial V} X_1 \mathbf{v}_1 \cdot \hat{\mathbf{n}}_{\partial V} \mathrm{d}S = 0}$$

- Example: 2D rectangular mesh cell
  - 3D case analog (6 faces instead of 4)

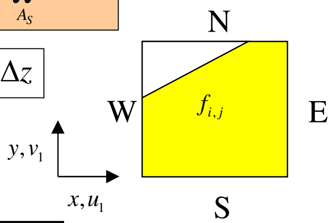


Derivation of f – equation in integral form

$$\oint\!\!\oint_{\partial V} X_1 \mathbf{v}_1 \cdot \hat{\mathbf{n}}_{\partial V} \mathrm{d}S = \iint_{A_E} X_1 u_1 \mathrm{d}S - \iint_{A_W} X_1 u_1 \mathrm{d}S + \iint_{A_N} X_1 v_1 \mathrm{d}S - \iint_{A_S} X v_1 \mathrm{d}S$$

$$V = \Delta x\, \Delta y\, \Delta z \qquad A_E = A_W = \Delta y\, \Delta z \qquad A_N = A_S = \Delta x\, \Delta z$$

$$\overline{X_1 u_1}^{A_E} \equiv \frac{1}{A_E} \iint_{A_E} X_1 u_1 \mathrm{d}S$$



$$\Rightarrow f^{n+1}_{i,j,k} = f^{n}_{i,j,k} + \Delta t \left(\frac{\overline{X_1 u_1}^{A_W} - \overline{X_1 u_1}^{A_E}}{\Delta x} + \frac{\overline{X_1 v_1}^{A_S} - \overline{X_1 v_1}^{A_N}}{\Delta y} \right)$$

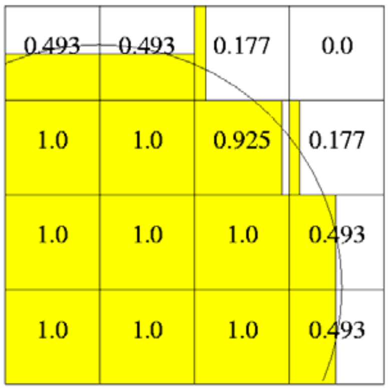
- For evaluation of this equation information on the velocities and phase distribution at the faces of the mesh cells is required
- Advantage: VOF method conserves exactly volume and mass

Reconstruction of phase distribution

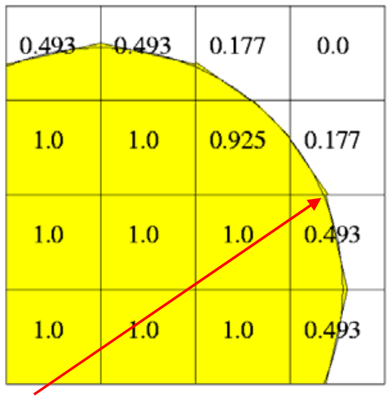
- Two concepts for reconstruction of position and orientation of interface in two-phase mesh cells ($0 < f < 1$)
- Simple Line Interface Calculation (SLIC)
  - The interface is oriented parallel to the face of a mesh cell
  - To which mesh face depends on neighboring mesh cells
- Piecewise Linear Interface Calculation (PLIC)
  - The interface in a mesh cell is approximated by a plane
  - The orientation of the plane is arbitrary
  - Problem: planes in neighboring mesh cells are not continuous

Example: reconstruction of circular arc

SLIC



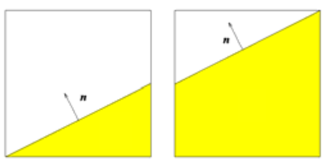
PLIC



Linear elements are in general discontinous at cell faces!

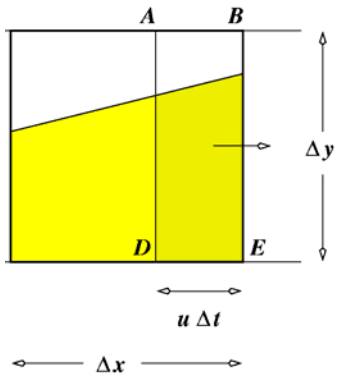
PLIC: computation of normal vector

- Mathematical exact relation: $\boxed{\hat{\mathbf{n}}_1 = \delta\left(\mathbf{x}-\mathbf{x}_i\right)\nabla X_1}$
- Approximation after volume averaging: $X_1 \approx f \quad \Rightarrow \quad \boxed{\hat{\mathbf{n}}_1 = \dfrac{\nabla f}{\left|\nabla f\right|}}$
- There exists a large number of PLIC reconstruction schemes for determining the unit normal vector from the discrete f values
- When the normal vector is known, the plane is “shifted” so that the liquid volume under the interface agrees with $f_{i,j,k}$



Advection step

- Two ways to compute the flux across mesh cell faces
- “Operator-Split“ method
  - For each coordinate direction a separate advection step is performed
  - After each advection step a reconstruction step follows
  - Thus 3 reconstruction steps per time step
- “Unsplit“ method
  - Only one reconstruction step per time step is performed
  - The same fluid volume may be advected twice or triple



Continuous surface force model

Idea of Brackbill et al. (1992):

Replace surface tension force acting on surface element

$$\boxed{\mathbf{F}_{\mathrm{sa}}(\mathbf{x}_{\mathrm{s}}) = \sigma\kappa(\mathbf{x}_{\mathrm{s}})\hat{\mathbf{n}}_1(\mathbf{x}_{\mathrm{s}})}$$

by volume force $\mathbf{F}_{\mathrm{sv}}(\mathbf{x})$ so that: $\boxed{\lim_{h\to 0}\iiint_{\Delta V}\mathbf{F}_{\mathrm{sv}}(\mathbf{x})\mathrm{d}V = \iint_{\Delta A}\mathbf{F}_{\mathrm{sa}}(\mathbf{x}_{\mathrm{s}})\mathrm{d}A}$

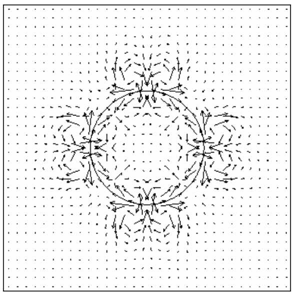
Result: $\boxed{\mathbf{F}_{\mathrm{sv}}(\mathbf{x}) = \sigma\kappa(\mathbf{x})\frac{\nabla\tilde{c}}{[c]}}$

$\tilde{c}$ is a smoothed “color function” and $[c]=c_1\text{-}c_2$ is the jump of c across the interface

For VOF method: $\boxed{\mathbf{F}_{\mathrm{sv}}(\mathbf{x}) \propto \sigma\kappa\nabla f}$ and $\boxed{\kappa = -\nabla\cdot\hat{\mathbf{n}}_1 = -\nabla\cdot\frac{\nabla f}{|\nabla f|}}$

Continuous surface force model

- Smoothing is necessary to minimize "spurious currents"
  - Consider a spherical bubble at zero gravity
  - Due to the discrete representation, the surface tension and pressure force are not in equilibrium and induce an artificial flow field = "spurious currents"
  - The intensity of the spurious currents depends on the Laplace number

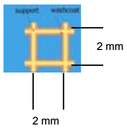


$$La \equiv \frac{\sigma \rho_L d_{\text{bubble}}}{\mu_L^2}$$

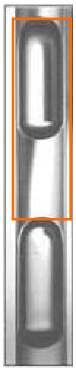
Example for VOF computations: Bubble train flow

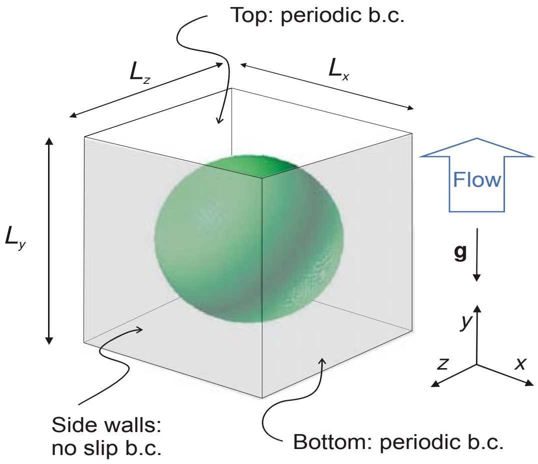
- Enhanced heat/mass transfer in devices with miniaturized channels such as micro bubble column and monolith reactors
- Goal: Evaluate performance of commercial CFD codes for interfacial simulation of gas-liquid flows in small channels
  - STAR-CD 4.0
  - ANSYS CFX 10.0
  - FLUENT 6.2.16
- Simulations of air/silicon oil bubble-train flow in a square mini-channel were surface tension forces are predominant
- Compare results with those of in-house code TURBIT-VOF which is already verified by experimental data

Numerical set-up for TURBIT-VOF, CFX and STAR-CD



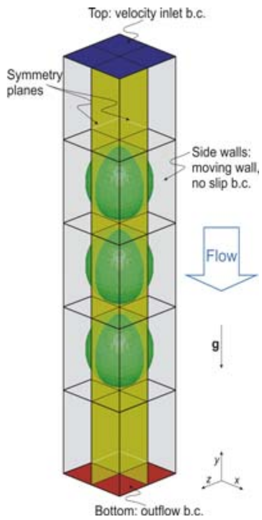
- Consideration of one unit cell in fixed frame of reference
- Use of periodic boundary conditions at top and bottom
- $L_x = L_y = L_z = 2$ mm





Numerical set-up for FLUENT

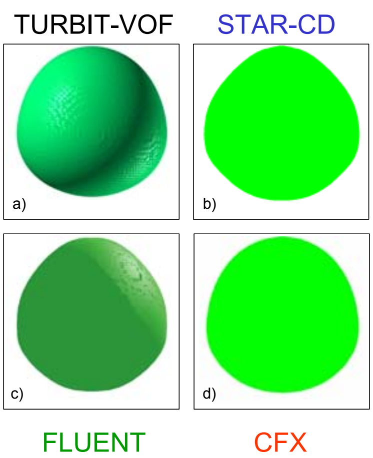
- FLUENT does not allow to use VOF method in combination with periodic boundary conditions
- Therefore simulations are performed in <u>moving frame of reference</u>
- Domain: 1 mm × 10 mm × 1 mm
- Downward wall velocity corresponds to terminal bubble velocity of TURBIT-VOF

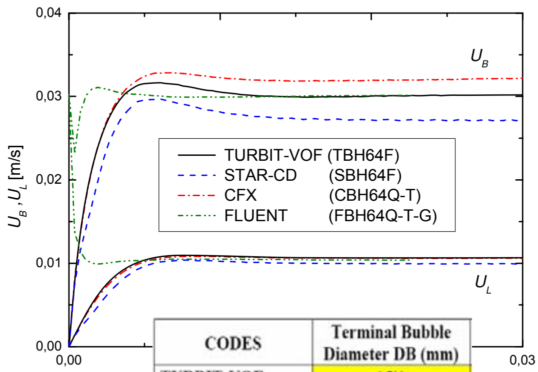


VOF methods in codes

- STAR-CD 4.0
  - VOF method without interface reconstruction
  - *f*-equation is solved by high order difference scheme
- CFX 10.0
  - Use of homogeneous model with surface tension force
  - *f*-equation is solved by high order difference scheme
- FLUENT 6.2
  - Solution of *f*-equation with high order difference scheme
    - Euler-explicit
    - Implicit
  - or, reconstruction of interface with
    - PLIC method (“Geo-reconstruct”)
    - SLIC method (“Donor-acceptor”)
- TURBIT-VOF (in-house code)
  - Reconstruction of interface by PLIC method

Bubble train flow case 1: Buoyancy driven flow

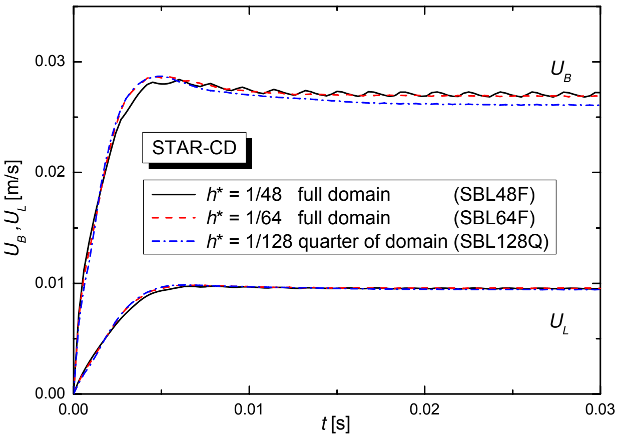




CODES	Terminal Bubble Diameter DB (mm)
TURBIT-VOF	1.711
STAR-CD	1.756
CFX	1.704
FLUENT	1.709

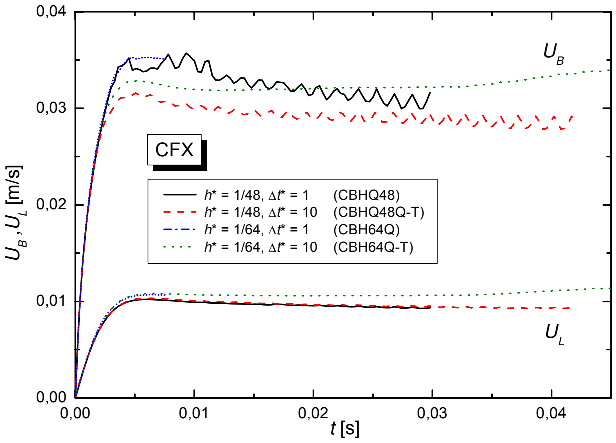
For FLUENT pressure drop is output and its value is -0.7 Pa
For other codes periodic pressure is input and its value is -0 Pa

Grid refinement study for STAR-CD



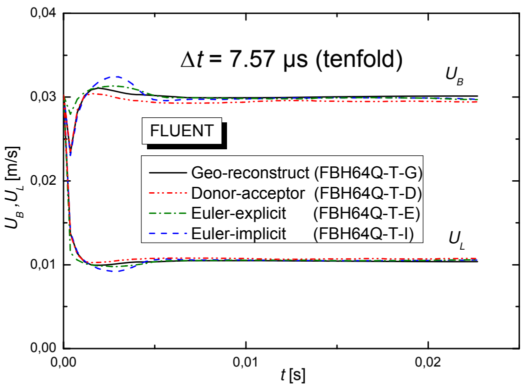
- Results do slightly depend on mesh size
- Refining the grid results in stronger underestimation of bubble velocity as compared to FLUENT and TURBIT-VOF

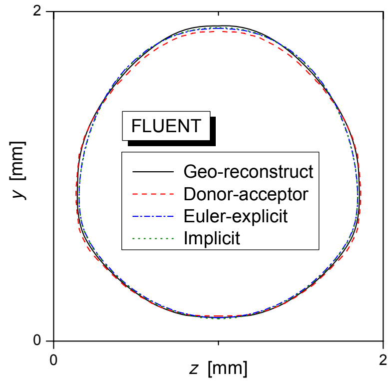
Grid and time step study for CFX



- Results depend on time step width (for same Δx)
- Results depend on mesh size (for same Δt)

Different VOF methods in FLUENT

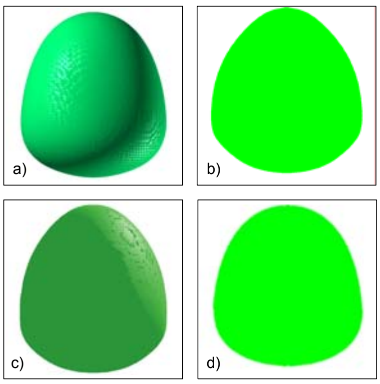




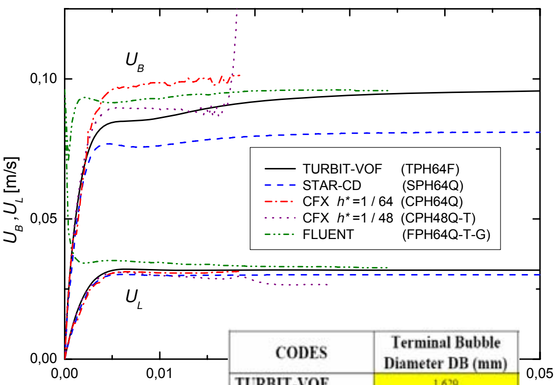
- „Geo-reconstruct“ scheme is almost independent from Δx and Δt

Bubble train flow case 2: Pressure driven flow

TURBIT-VOF STAR-CD



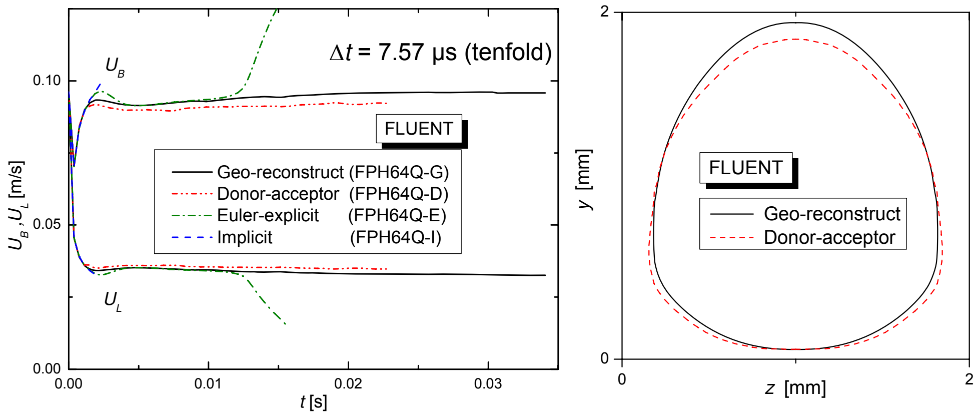
FLUENT CFX



CODES	Terminal Bubble Diameter DB (mm)
TURBIT-VOF	1.629
STAR-CD	1.693
CFX	1.641
FLUENT	1.634

For FLUENT Periodic pressure is output and its value is -21.5 Pa
For rest of codes Periodic pressure is input and its value is -18 Pa

Different VOF methods in FLUENT



- Only VOF methods with reconstruction result in "bubble train flow"

Conclusions regarding VOF methods

- VOF methods based on piecewise linear interface reconstruction (PLIC) give consistent results
- Higher order difference scheme methods have deficiencies
  - Unphysical results for decrease of gas holdup (CFX,STAR-CD)
  - Strong influence time step width (CFX)
  - Influence of grid size (CFX, STAR-CD)
  - Numerical diffusion may lead to artificial coalescence (all codes)
- For the commercial CFD codes the recommended PLIC reconstruction scheme is only available in FLUENT

Level-set method

- The level-set method is based on local equations (usually no volume averaging is performed)
- Interface is represented by a smooth function ϕ

$$S_\mathrm{i} = \{\mathbf{x} \mid \phi(\mathbf{x},t) = 0\}$$

$$\phi(\mathbf{x},t) = \begin{cases} > 0 & \text{for} \quad \mathbf{x} \in \Omega_1 \\ = 0 & \text{for} \quad \mathbf{x} \in S_\mathrm{i} \\ < 0 & \text{for} \quad \mathbf{x} \in \Omega_2 \end{cases}$$

- In practice ϕ is the signed distance to the interface

Level-set method

- Advection equation for ϕ

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

  – Because ϕ is a smooth function this equation can be solved by standard finite difference schemes

- Computation of density and viscosity

$$\rho(\mathbf{x}) = \rho_1 + (\rho_1 - \rho_2) H_\varepsilon(\phi(\mathbf{x})) \qquad \mu(\mathbf{x}) = \mu_1 + (\mu_1 - \mu_2) H_\varepsilon(\phi(\mathbf{x}))$$

$$H_\varepsilon \equiv \begin{cases} 0 & \text{if } \phi < -\varepsilon \\ \dfrac{\phi+\varepsilon}{2\varepsilon} + \dfrac{\sin(\pi\phi/\varepsilon)}{2\pi} & \text{if } |\phi| \le \varepsilon \\ 1 & \text{if } \phi > \varepsilon \end{cases}$$

H_ε = smoothed Heaviside function
ε = O(Δx)

Level-set method

- Surface tension force is modeled as body force

$$\mathbf{f}_\sigma = \sigma\kappa\nabla\phi\delta_\varepsilon(\phi)$$

$$\kappa = -\nabla\cdot\hat{\mathbf{n}}_1 = -\nabla\cdot\left(\frac{\nabla\phi}{|\nabla\phi|}\right)$$

$$\delta_\varepsilon(\phi) = \mathrm{d}H_\varepsilon(\phi)/\mathrm{d}\phi = \begin{cases} \dfrac{1+\cos(\pi\phi/\varepsilon)}{2\varepsilon} & \text{if } |\phi|<\varepsilon \\ 0 & \text{otherwise} \end{cases}$$

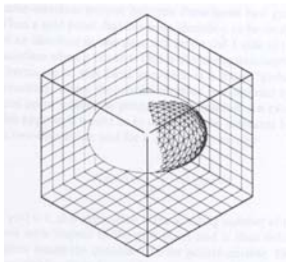
In literature several approximations for the smoothed delta function exist

Level-set method

- Advantages
  - ϕ - equation can be discretized by finite difference schemes
  - There is no complicated interface reconstruction required as in VOF
  - Interface is represented as continuous surface
  - Coalescence and break-up are easy to handle
- Disadvantage
  - Volume respectively mass are not exactly conserved
  - The distance function ϕ must be re-computed after each time step

Front-tracking method

- Method is based on local equations (no volume averaging)
- Method uses two different grids
  - Fixed structured grid for momentum equation (Euler grid)
  - Moving unstructured grid for the representation of the interface
- Description of interface
  - Marker particles are assigned to interface
  - Velocity is interpolated from the Euler grid to the position of marker particles
  - The marker particles are advected
  - New position of all marker particles gives updated shape of interface



Source: G. Tryggvason

Front-tracking method

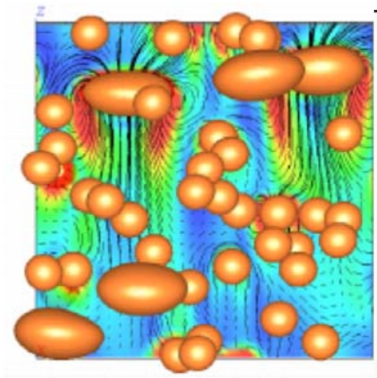
- Surface tension
  - Analytical evaluation of the normal vector from bubble shape

$$\mathbf{F}_\sigma = \iint_{\delta \mathcal{A}} \sigma\kappa \hat{\mathbf{n}}_1 \mathrm{d}S = \iint_{\delta \mathcal{A}} \sigma \left(\hat{\mathbf{n}}_1 \times \nabla\right) \times \hat{\mathbf{n}}_1 \mathrm{d}S = \oint_{\mathcal{L}} \sigma \mathbf{t} \times \hat{\mathbf{n}}_1 \mathrm{d}C$$

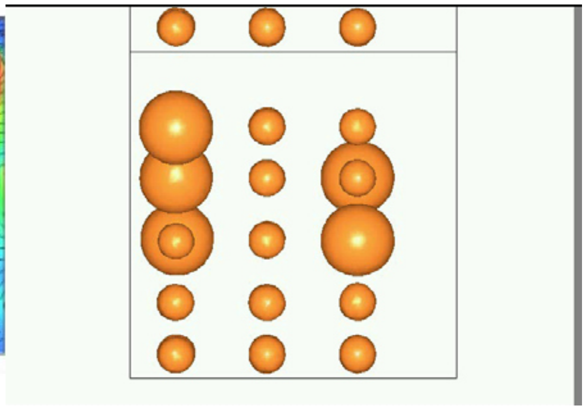
- Advantages of front-tracking method
  - Accurate representation of interface
  - Powerful method; simulations for more than 200 bubbles were performed
- Disadvantages
  - Coalescence / break-up are difficult to handle
  - Complex algorithm for unstructured grid (marker points must be added and removed)

Front-tracking method: Example

- Rise of 40 small and 5 large bubbles in a fully periodic domain



Streamlines and contour lines of vorticity



Source: Göz, Bunner, Sommerfeld & Tryggvason 2002

Summary

- Within the academic community there are much more models for multiphase flows under development than could be covered here
- Important models available in leading CFD codes
  - Euler-Lagrange model is powerful for sprays, but only for low void fractions
  - Two-fluid model is powerful and general method, but relies on adequate models for interfacial exchange processes (o.k. for bubbly flows)
  - VOF method with interface reconstruction is powerful for stratified and partly for disperse flows but requires adequate resolution of interface curvature
- The capabilities of commercial CFD codes to model turbulence in multiphase flows (stratified and disperse) are still very limited