TOPIC 2

Mechanics

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2.1. Thermal-hydraulics

2.1.2 Two phase flow modelling and simulation

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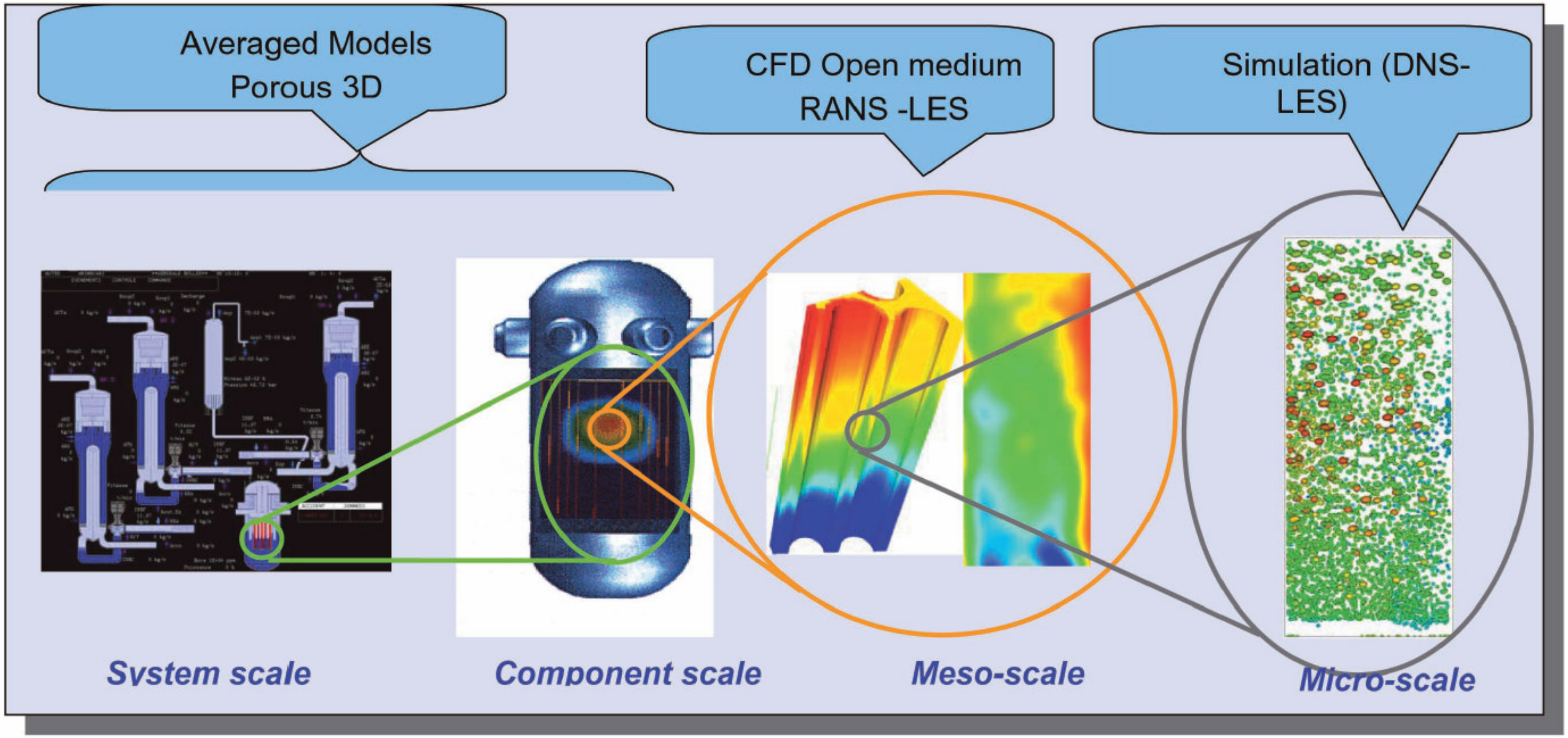
Content

- Introduction
  - CFD in nuclear engineering
  - Gas-liquid two phase flows
- Governing equations
  - Local equations
  - Averaging and closure problem
- Models for interpenetrating continua
  - Homogeneous model
  - Algebraic slip model and drift-flux model
  - Two-fluid model and its advanced variants
- Final remarks

Multi-scale analysis of reactor thermal hydraulics



D. Bestion *Nucl Eng Techn* **42** (2010) 608

CFD/CMFD* codes versus 1D codes

	System codes/1D codes	CFD codes
Codes	Athlet, Cathare, Relap, …	CFX, Fluent, Neptune, Star-CD, Trans-AT, …
Geometry	Very much simplified	Arbitrary complex
Control volume	Large	Arbitrary small
Mathematical description	Networks of 1D/0D cells; Partial differential eqs (1D)	Partial differential equations (2D/3D)
Closure relations	Empirical correlations from large experimental data bases	Mechanistic i.e. based on clear physical phenomena

* CMFD = Computational *Multi*-Fluid Dynamics

Need for CFD in nuclear reactor safety

- Where the geometry is 2D/3D
  - Upper and lower plenum
  - Downcomer
  - Reactor core
  - …
- Where the physics is 2D/3D
  - Natural circulation
  - Mixing
  - Stratification
  - …
- Bestion list 26 two-phase flow NRS issues that may benefit from CFD investigations
  - Bestion *Nucl Eng Techn* **42** (2010) 365

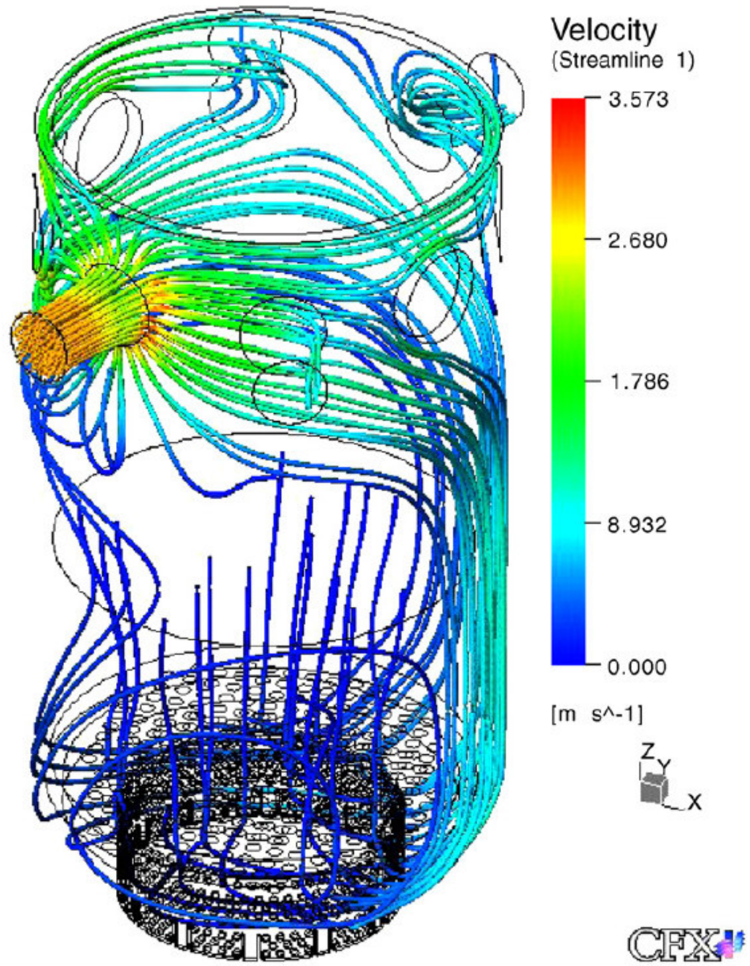


Fig. from Rohde et al. *Nucl Eng Des* **237** (2007) 1639

Essential steps in a CFD simulation

1. Think about the essential physics of the problem
2. Select governing equations / simulation method
3. Specify physical models

In this lecture

4. Decide on computational domain
5. Generate grid
6. Specify inlet/outlet/boundary conditions
7. Specify discretization scheme and iterative solver
8. Solve the flow problem (steady state or transient)
9. Analyze results (post processing)
10. Are results valid? If not revisit the above topics …

It is the <u>duty of the user</u> to check whether the results are an appropriate approximation of the physical problem!

Flow regimes in a vertical pipe

- Methods and models must account for the **flow regime** of the gas-liquid two-phase flow

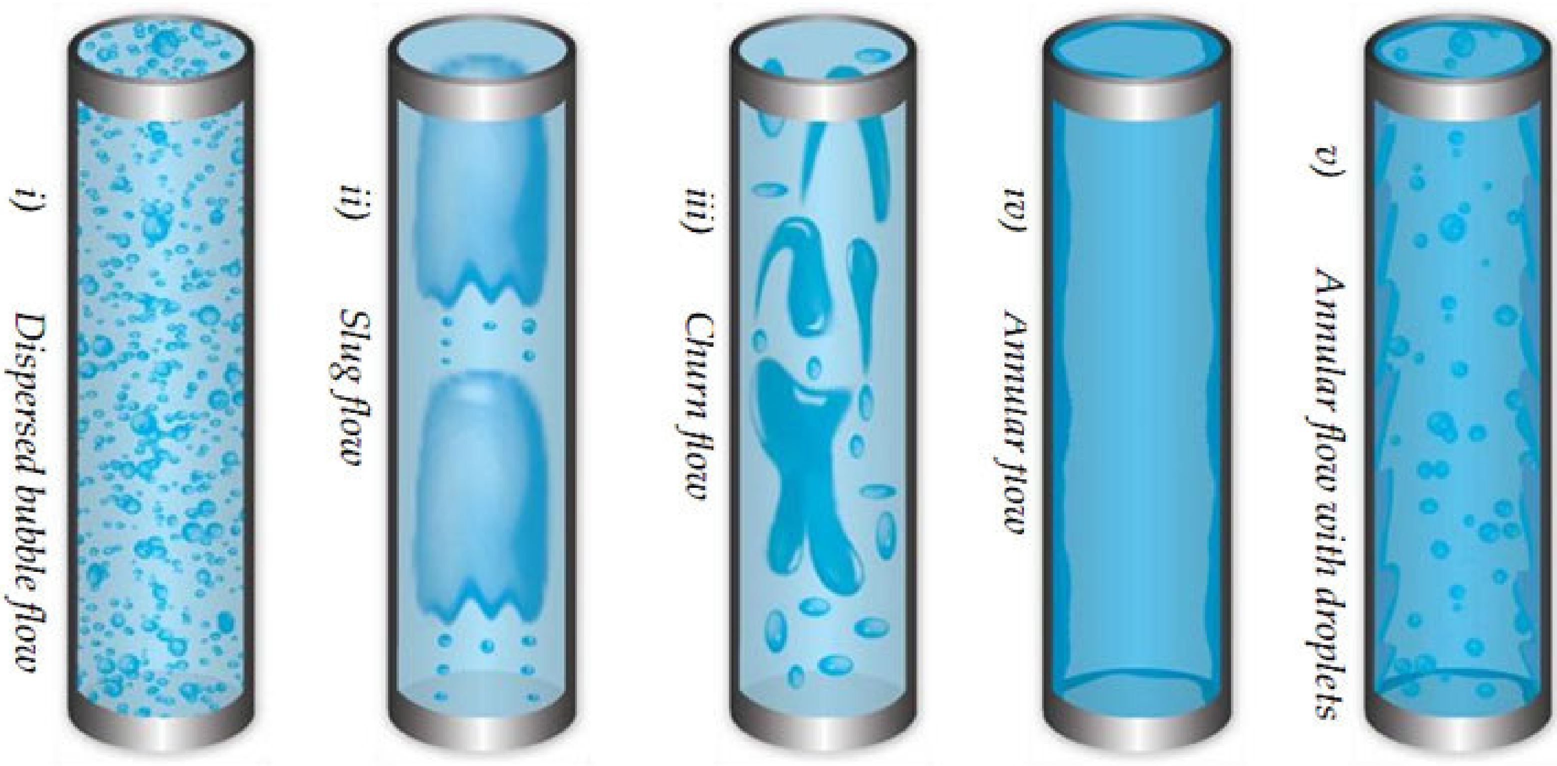


Fig. from O. Bratland „Pipe Flow 2: Multi-phase Flow Assurance” (http://www.drbratland.com/index.html)

Flow regime map for horizontal pipe

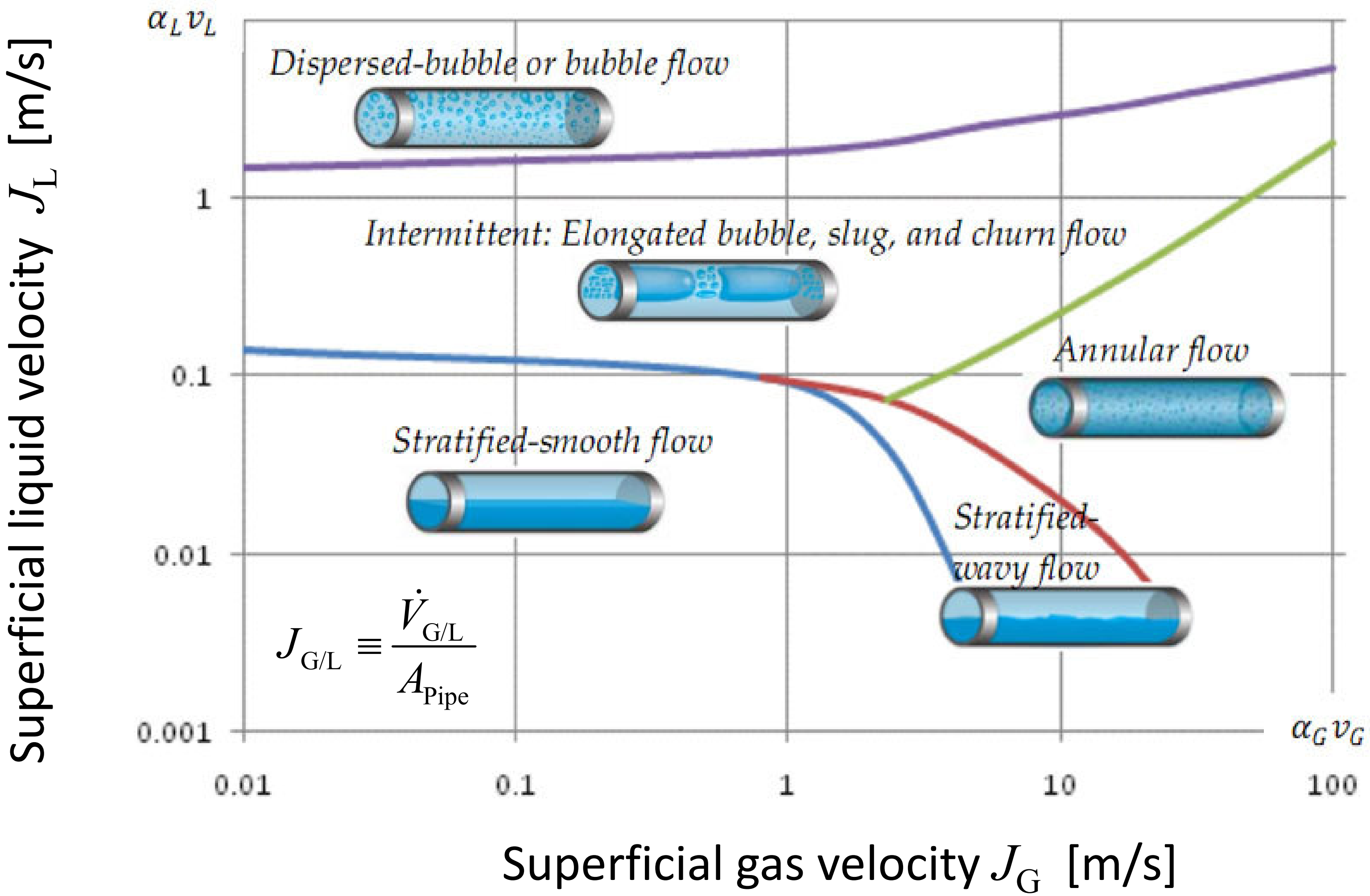
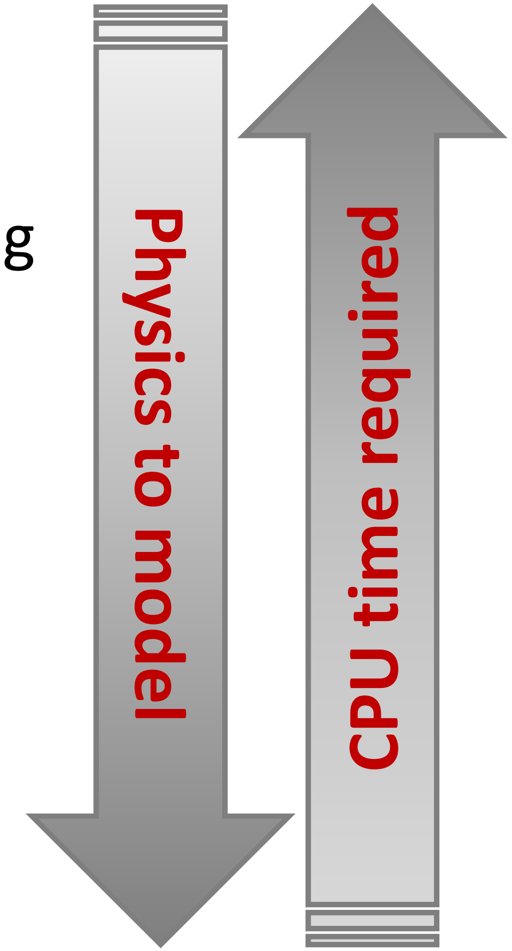


Fig. from O. Bratland „Pipe Flow 2: Multi-phase Flow Assurance" (http://www.drbratland.com/index.html)

CFD methods for gas-liquid flows

- Interface resolving methods
  - For disperse and free surface flows
  - Volume-of-fluid, Level set, Front tracking
- Euler-Lagrange method
  - For disperse flows (bubbles/drops)
  - Point-particle approach
- Interpenetrating field approach
  - Suitable for <u>all</u> flow regimes
  - Homogenous model, algebraic slip m., two-fluid model (Euler-Euler model)

Models covered in this lecture



The model approach depends on the <u>scales that shall be resolved</u>

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The exact eqs in each bulk phase

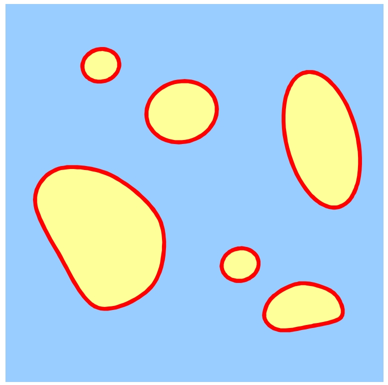
Conservation of mass, momentum, energy

Interface Γ

Fluid 1 (liquid)

Fluid 2 (gas)

$$\left.\begin{aligned} \frac{\partial \rho_1}{\partial t} + \nabla \cdot \rho_1 \mathbf{v}_1 = 0 \\ \frac{\partial \left(\rho_1 \mathbf{v}_1 \right)}{\partial t} + \nabla \cdot \left(\rho_1 \mathbf{v}_1 \mathbf{v}_1 \right) = -\nabla p_1 + \nabla \cdot \mathbb{T}_1 + \rho_1 \mathbf{g} \\ \frac{\partial \left(\rho_1 h_1 \right)}{\partial t} + \nabla \cdot \left(\rho_1 h_1 \mathbf{v}_1 \right) = \frac{\mathrm{D}_1 p_1}{\mathrm{D}t} - \nabla \cdot q_1 + \mathbb{T}_1 : \nabla \mathbf{v}_1 + Q_1 \end{aligned} \right\} \mathbf{x} \in \Omega_1 (t)$$



$$\left.\begin{aligned} \frac{\partial \rho_2}{\partial t} + \nabla \cdot \rho_2 \mathbf{v}_2 = 0 \\ \frac{\partial \left(\rho_2 \mathbf{v}_2 \right)}{\partial t} + \nabla \cdot \left(\rho_2 \mathbf{v}_2 \mathbf{v}_2 \right) = -\nabla p_2 + \nabla \cdot \mathbb{T}_2 + \rho_2 \mathbf{g} \\ \frac{\partial \left(\rho_2 h_2 \right)}{\partial t} + \nabla \cdot \left(\rho_2 h_2 \mathbf{v}_2 \right) = \frac{\mathrm{D}_2 p_2}{\mathrm{D}t} - \nabla \cdot q_2 + \mathbb{T}_2 : \nabla \mathbf{v}_2 + Q_2 \end{aligned} \right\} \mathbf{x} \in \Omega_2 (t)$$

ρ_k = density $(k=1,2)$

$\mathbf{v}_k$ = velocity field

p_k = pressure

$\mathbb{T}_k$ = viscous stress tensor

h_k = enthalpy

q_k = heat flux

Q_k = internal heat source

Jump conditions at the interface*

- Kinematic condition

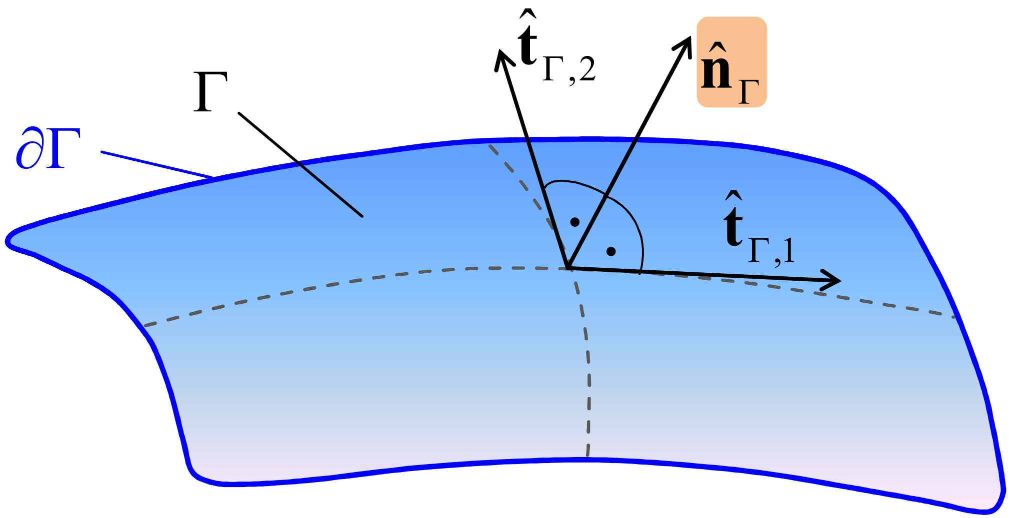
$$(\mathbf{v}_1 - \mathbf{v}_2) \cdot \hat{\mathbf{n}}_\Gamma = 0$$

unit normal vector to interface (pointing in phase 1)

- Dynamic condition (force balance at a surface element Γ)

$$-(p_1 - p_2)\hat{\mathbf{n}}_\Gamma + (\mathbb{T}_1 - \mathbb{T}_2) \cdot \hat{\mathbf{n}}_\Gamma = 2H\sigma\hat{\mathbf{n}}_\Gamma + \nabla_\Gamma \sigma$$

coefficient of surface tension



Newtonian fluid:

$$\mathbb{T}_k = 2\mu_k \mathbb{D}_k$$

$$\mathbb{D}_k \equiv \frac{1}{2}\left[\nabla \mathbf{v}_k + (\nabla \mathbf{v}_k)^{\mathrm{T}}\right]$$

- Heat balance

$$(\mathbf{q}_1 - \mathbf{q}_2) \cdot \hat{\mathbf{n}}_\Gamma = 0$$

* here for simplicity without phase change

Steam-water flow in hot-leg of PWR

TOPFLOW facility at HZDR

- pressure up to 50 bar
- temperature up to 264°C

Reflux-condenser mode: investigation of counter-current flow limitation (CCFL) in the „hot leg“ of a Konvoi PWR (scale 1:3)

It is neither possible nor meaningful to perform a simulation which resolves all details of the interface/flow

⇒ <u>Need for averaging</u> (smoothing)

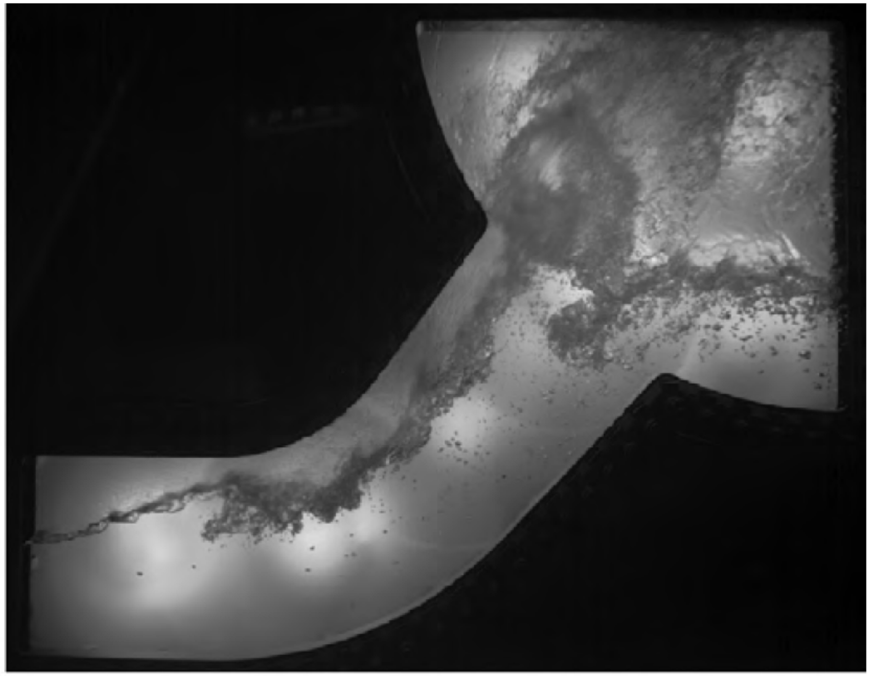
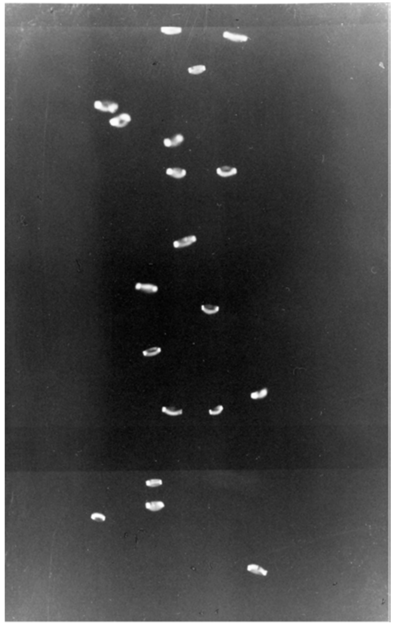


Illustration of time averaging

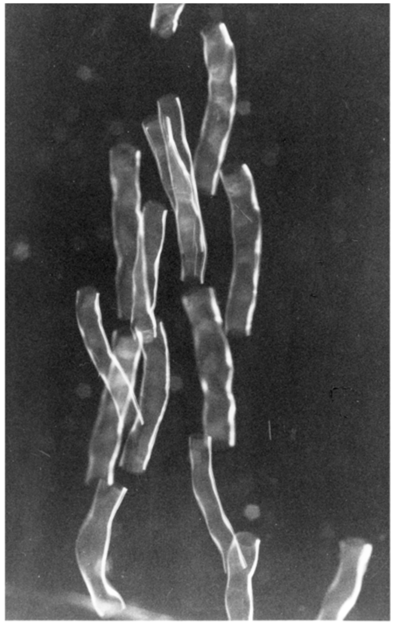
Instantaneous view

At any point there exists either phase 1 or phase 2



Time averaged view

The phases coexist and form ***"interpenetrating continua"***

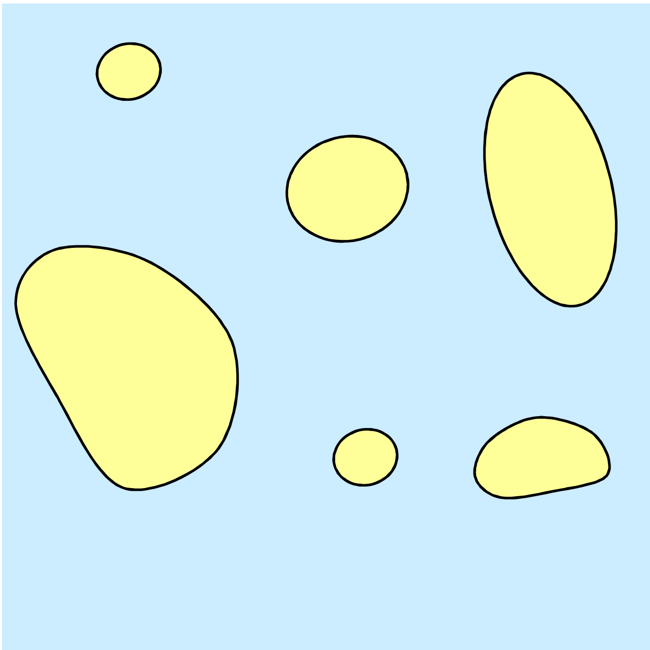


In the sequel we consider not time but volume averaged equations (all major commercial CFD codes are finite volume codes)

Definitions for volume averaging

Phase indicator function: $X_k(\mathbf{x},t) \equiv \begin{cases} 1, & \text{if } \mathbf{x} \in \Omega_k(t) \\ 0, & \text{else} \end{cases}$

$X_1 + X_2 = 1$



Definitions for volume averaging

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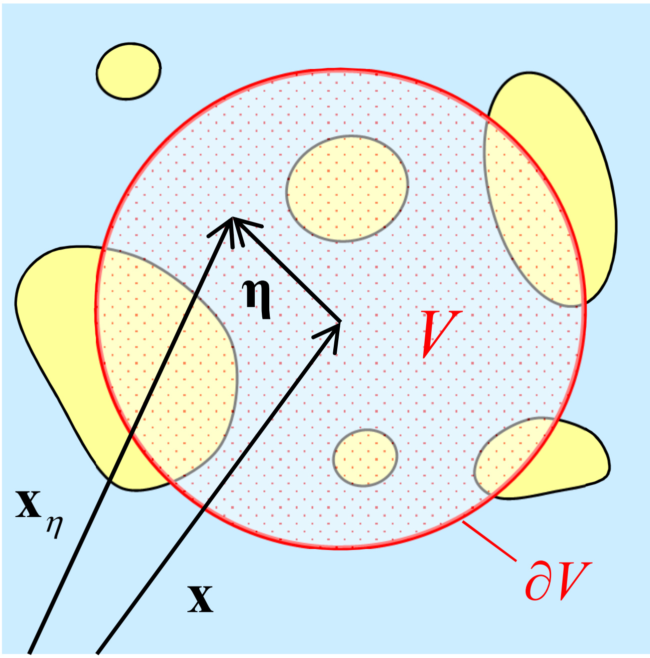
$X_1 + X_2 = 1$

Averaging volume V with boundary ∂V



Volume of phase k in V:

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

Volume fraction of phase k in V:

$$\alpha_k \equiv \frac{V_k}{V}, \quad 0 \le \alpha_k \le 1, \quad \alpha_1 + \alpha_2 = 1$$

Phase average of variable φ_k in V:

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

Derivation of volume-averaged eqs

1. Take the two sets of local conservation equations (valid only in the respective phase)
2. Multiply by respective phase indicator function $\Rightarrow$ equations become valid in <u>entire</u> domain
3. Integrate over a control volume (in practice the control volume corresponds to a mesh cell)
4. Apply the Gauss and Leibniz rule (volume average and time/space derivative do <u>not</u> commute here)
5. Obtain two sets of "**interpenetrating**" volume-averaged conservation eqs valid in entire domain

Volume averaged momentum eqs

$$\frac{\partial \alpha_1 \rho_1 \overline{\mathbf{v}_1}^1}{\partial t} + \nabla \cdot (\alpha_1 \rho_1 \overline{\mathbf{v}_1 \mathbf{v}_1}^1) = -\nabla \alpha_1 \overline{p_1}^1 + \alpha_1 \rho_1 \mathbf{g} + \nabla \cdot \alpha_1 \overline{\mathbb{T}_1}^1 + \mathbf{M}_1$$

$$\frac{\partial \alpha_2 \rho_2 \overline{\mathbf{v}_2}^2}{\partial t} + \nabla \cdot (\alpha_2 \rho_2 \overline{\mathbf{v}_2 \mathbf{v}_2}^2) = -\nabla \alpha_2 \overline{p_2}^2 + \alpha_2 \rho_2 \mathbf{g} + \nabla \cdot \alpha_2 \overline{\mathbb{T}_2}^2 + \mathbf{M}_2$$

Non-linear terms: $\rho_k \overline{\mathbf{v}_k \mathbf{v}_k}^k = \rho_k \overline{\mathbf{v}_k}^k \overline{\mathbf{v}_k}^k - \underbrace{\rho_k \overline{\mathbf{v}'_k \mathbf{v}'_k}^k}_{\mathbb{T}_k^{\mathrm{sgs}}}$ $\mathbb{T}_k^{\mathrm{sgs}}$ = subgrid stress tensor

Momentum transfer term:

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

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

The two momentum equations are coupled by a jump condition which results from volume averaging of the dynamic condition at the interface

Closure problem (hydrodynamics)

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**

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Mass conservation phase 1	1
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Momentum conservation phase 1	3
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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
(turbulence model)	
Total	**15**

$\Rightarrow$ ***3 scalar or one vector equation is required for closure!***

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Three concepts for closure

- Homogeneous model
  - Assumption of mechanical and thermal equilibrium (phases have same velocity/temperature in CV)
- Algebraic slip (drift-flux) model
  - The relative velocity in the CV is modeled by an algebraic equation

Four equations:

- *mass liquid*
- *mass vapor*
- *momentum of mixture*
- *energy of mixture*

- Two-fluid (Euler-Euler) model
  - The momentum and energy transfer between the phases is modeled

Six equations:

- *mass, momentum & energy of liquid*
- *mass, momentum & energy of vapor*

Homogeneous model (HM)

- Closure assumption: $\overline{\mathbf{v}_1}^{1} = \overline{\mathbf{v}_2}^{2} = \mathbf{v}$
  - "Mechanical equilibrium"
- Summing up the two momentum equations
  - "Single field" momentum equation for two-phase mixture

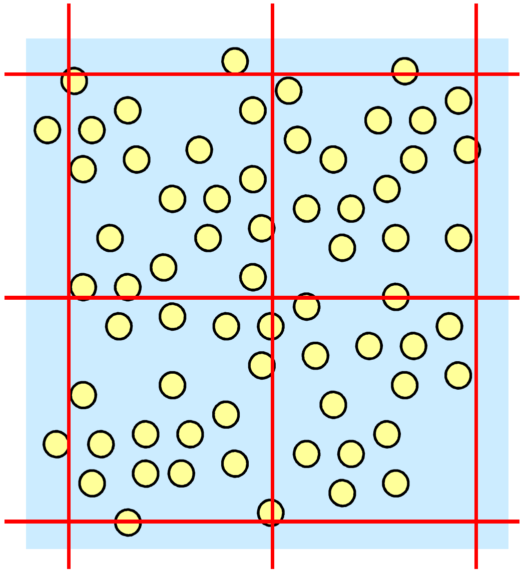
$$\frac{\partial \rho_{\mathrm{m}} \mathbf{v}}{\partial t} + \nabla \cdot \rho_{\mathrm{m}} \mathbf{v}\mathbf{v} = -\nabla p + \rho_{\mathrm{m}} \mathbf{g} + \nabla \cdot \mu_{\mathrm{m}} \left(\nabla \mathbf{v} + (\nabla \mathbf{v})^{\mathrm{T}} \right) + \frac{1}{V} \iint_{\Gamma \cap V} 2\sigma H \hat{\mathbf{n}}_{\Gamma} \, \mathrm{d}s$$

$$\rho_{\mathrm{m}} \equiv \alpha_1 \rho_1 + (1 - \alpha_1) \rho_2 \qquad \mu_{\mathrm{m}} \equiv \alpha_1 \mu_1 + (1 - \alpha_1) \mu_2$$

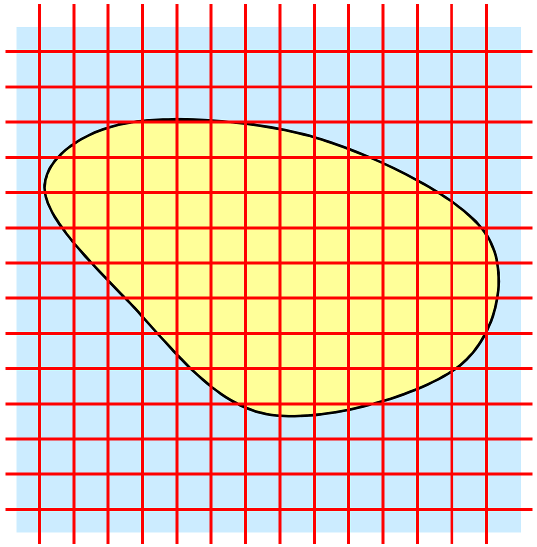
  - Density/viscosity vary in space and time depending on the local volume fraction $\alpha_1 = \alpha_1(\mathbf{x}, t)$
  - α_1 is obtained from solution of mass conservation eq. for phase 1
  - The surface tension term is often neglected

Applicability of homogeneous model

- Mechanical equilibrium can be a valid assumption for separate flow or disperse flow (*not buoyancy driven!*)
  - Fine dispersed or well separated depends on the size of the particle and that of the averaging volume/mesh cell



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



In almost all cells α_1=0 or α_1=1

1. No neglect of surface tension
2. Special scheme for solution of α_1 eq. (VOF, Level set)
3. Very fine grid

= ***Interface resolving simulation ("DNS")***

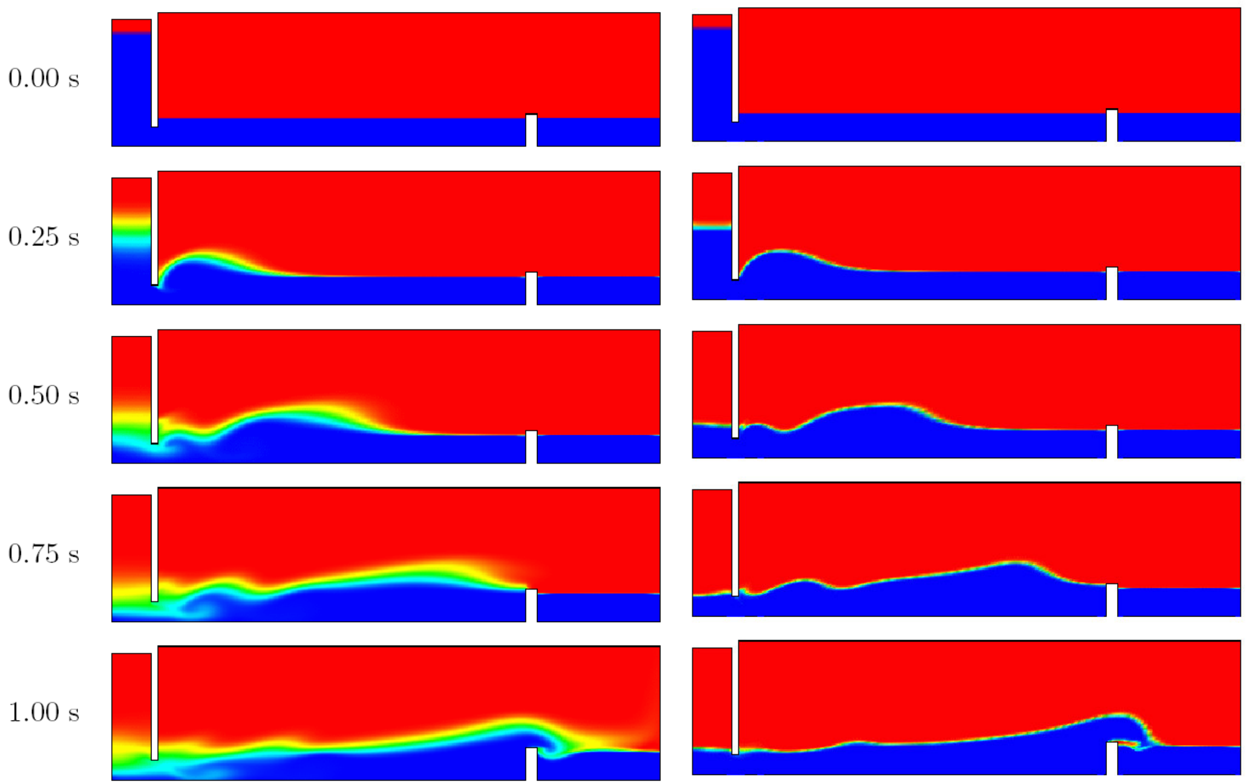
HM for 2D "dam break" problem*

- Code CFX 5.5
- Structured mesh with 19010 cells
- No surface tension
- Eqs are solved with two discretization schemes
- *Numerical diffusion* of upwind scheme smears the interface
- **Both, model <u>and</u> discr. scheme must be adequate for the physical problem!**

Liquid volume fraction field

red: $\alpha_1=0$ (gas), blue: $\alpha_1=1$ (water)

Upwind scheme (1st O.) High resolution scheme



* F. Menter, personal information

Algebraic slip model (ASM)

- Constitutive equation of the ASM
  - The relative velocity between the phases (slip velocity) is modeled by an algebraic relation

$$\mathbf{v}_\mathrm{r} \equiv \overline{\mathbf{v}_2}^{2} - \overline{\mathbf{v}_1}^{1} = \mathbf{v}_\mathrm{r}(\rho_1, \rho_2, \mu_1, \mu_2, \sigma, \alpha_1, \mathbf{v}_\mathrm{m}, d_\mathrm{p}, \ldots)$$

  - The continuity eqs and the mixture momentum eq include additional terms that depend on $\mathbf{v}_\mathrm{r}$
  - The HM is a special case of the ASM $(\mathbf{v}_\mathrm{r} = 0)$
  - The surface tension force is usually neglected
- Applicability: disperse flow only
  - Example: closure relation for bubbly flow

$$\mathbf{v}_\mathrm{r} = \begin{pmatrix} 0 \\ 0 \\ 20 \end{pmatrix} \mathrm{cm/s}$$

Drift-flux model (DFM)

- Closure by algebraic eq. for the disperse phase drift velocity
- Definitions of the drift velocities of the phases:

$$\mathbf{v}_{1\mathrm{j}} \equiv \overline{\mathbf{v}_1}^{1} - \mathbf{j}_\mathrm{m}, \quad \mathbf{v}_{2\mathrm{j}} \equiv \overline{\mathbf{v}_2}^{2} - \mathbf{j}_\mathrm{m} \quad \text{where} \quad \mathbf{j}_\mathrm{m} \equiv \alpha_1 \overline{\mathbf{v}_1}^{1} + \alpha_2 \overline{\mathbf{v}_2}^{2}$$

- Relation between drift velocities and relative velocity:

$$\mathbf{v}_{1\mathrm{j}} = -\alpha_2 \mathbf{v}_\mathrm{r}, \quad \mathbf{v}_{2\mathrm{j}} = \alpha_1 \mathbf{v}_\mathrm{r}$$

- The DFM is usually applied in its 1D form (obtained by area averaging over the channel cross-section)
- Constitutive relations for 1D DFM are available for various flow regimes (bubbly, slug, annular, stratified flow, ...)
  - see e.g. Ishii & Hibiki *Thermo-fluid dynamics of two-phase flow,* Springer, 2006

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Closure term in two-fluid model

- Interfacial transfer of momentum (and energy)
  - Integral is over that part of the interface that is in the CV

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

- Analogy : closed integral over entire surface area of bubble, drop, rigid particle of the *dynamic* pressure and normal viscous stress = ***hydrodynamic force***

$$\mathbf{F}_{\mathrm{hydr}} = \oiint_{\mathcal{A}_{\mathrm{p}}}\left[-p_{1,\mathrm{dyn}}\mathbb{I} + \mu_1\left(\nabla\mathbf{v}_1 + \left(\nabla\mathbf{v}_1\right)^{\mathrm{T}}\right)\right]\cdot\hat{\mathbf{n}}_\Gamma \mathrm{d}s$$

Hydrodynamic force on a rigid sphere

- Analytical solution for creeping flow (Stokes)

$$\mathbf{F}_{\text{hydr}} = \oiint_{\mathcal{A}_\text{p}} \left[-p_{1,\text{dyn}} \mathbb{I} + \mu_1 \left(\nabla \mathbf{v}_1 + \left(\nabla \mathbf{v}_1 \right)^\text{T} \right) \right] \cdot \hat{\mathbf{n}}_\Gamma \, \mathrm{d}s$$

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

- Generalization: $\mathbf{F}_{\text{hydr}} = \mathbf{F}_{\text{drag}} + \mathbf{F}_{\text{vm}} + \mathbf{F}_{\text{hist}} + \mathbf{F}_{\text{lift}} + \ldots$

Linear superposition of forces

$\mathcal{A}_\text{p}$ = particle surface area

$\mathcal{V}_\text{p}$ = particle volume

$V_\text{p} = |\mathbf{V}_\text{p}|$ = particle velocity

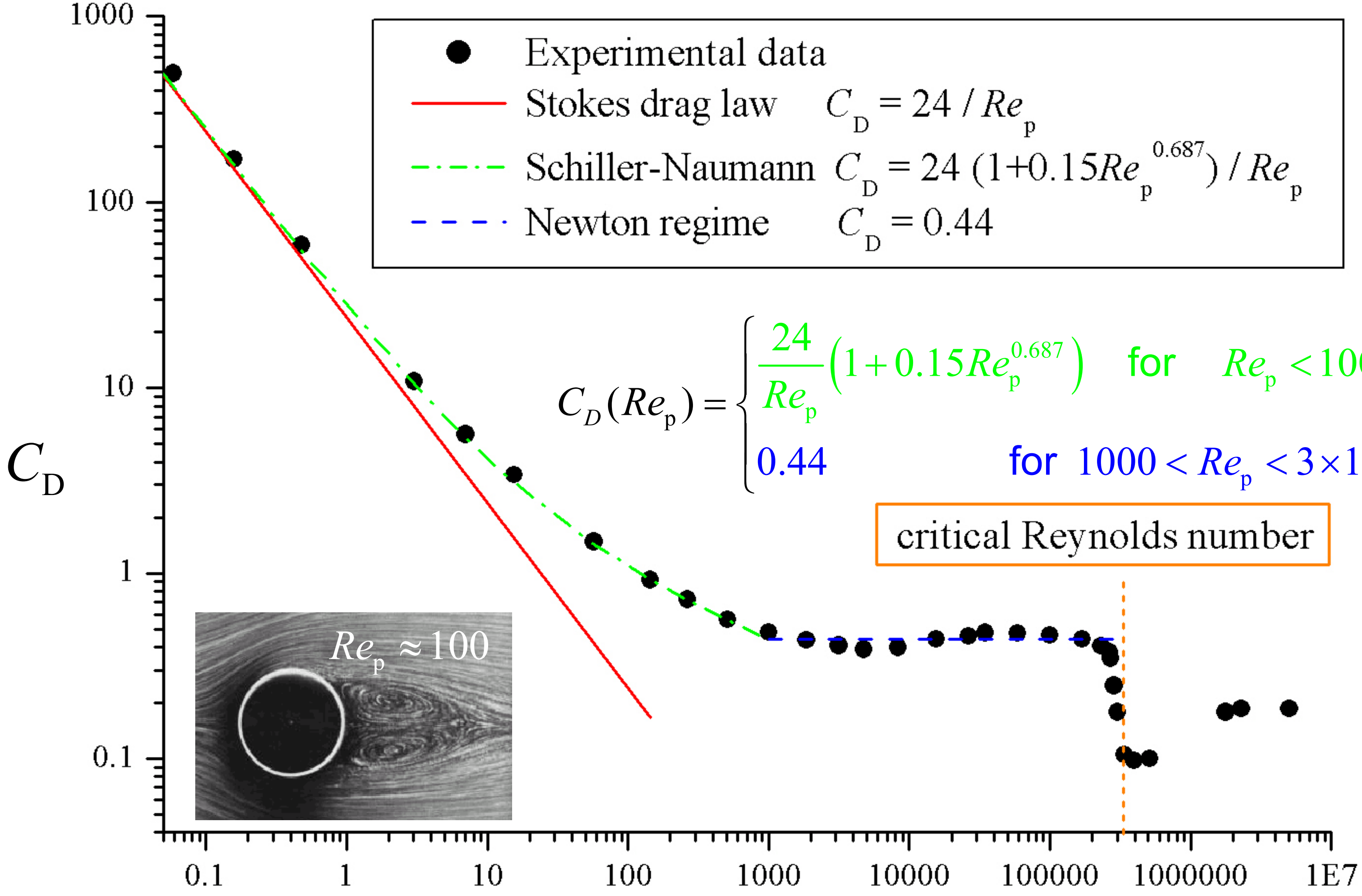
A_p = particle cross-sectional area

C_D = drag coefficient

$$\mathbf{F}_{\text{drag}} = -\frac{1}{2}\rho_1 A_\text{p} C_\text{D} \mathbf{U}_{\text{rel}} |\mathbf{U}_{\text{rel}}|$$

$$\mathbf{U}_{\text{rel}} = \mathbf{V}_\text{p} - \mathbf{v}_{\text{liquid}}$$

Drag coefficient for a rigid sphere

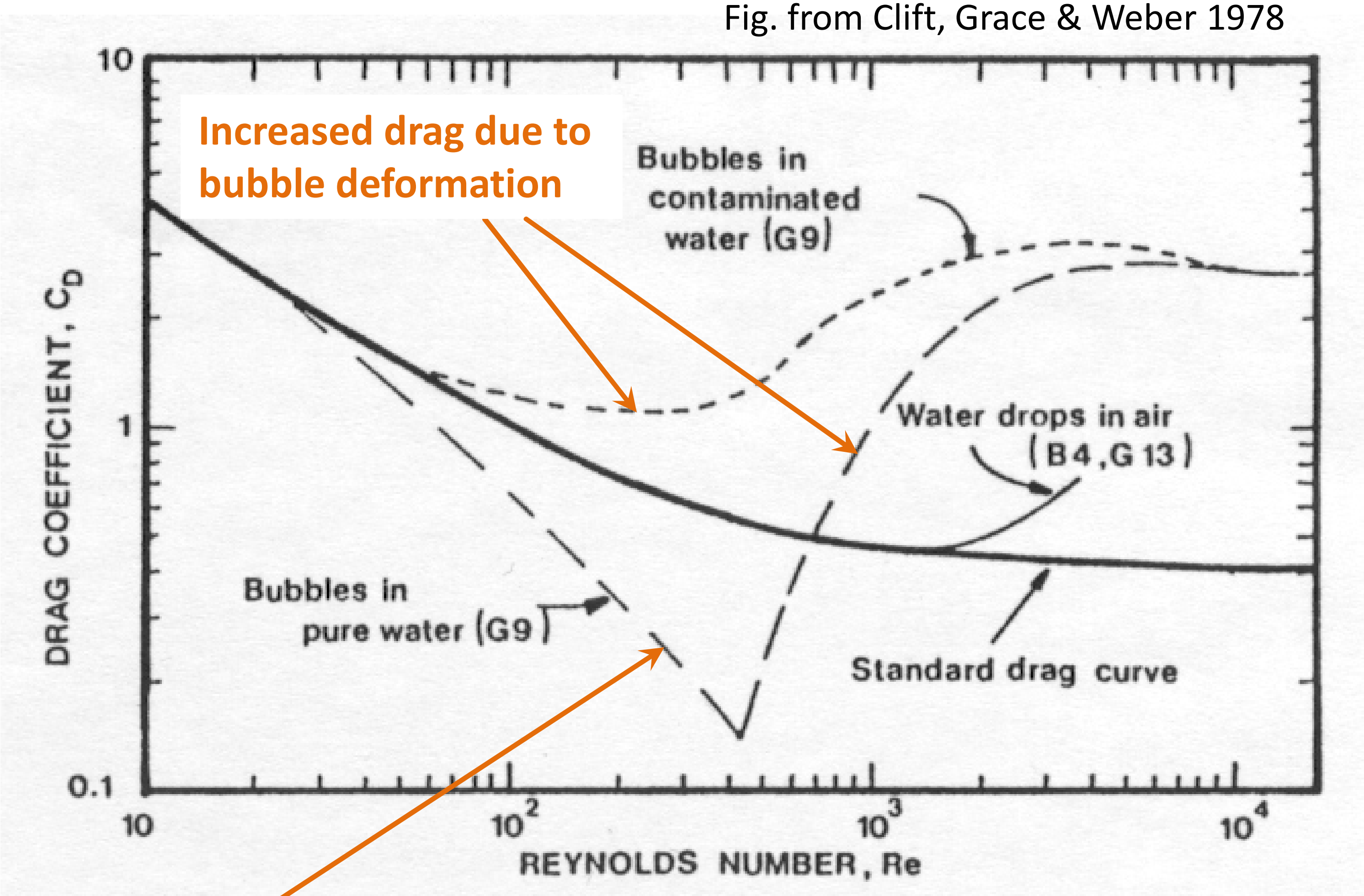


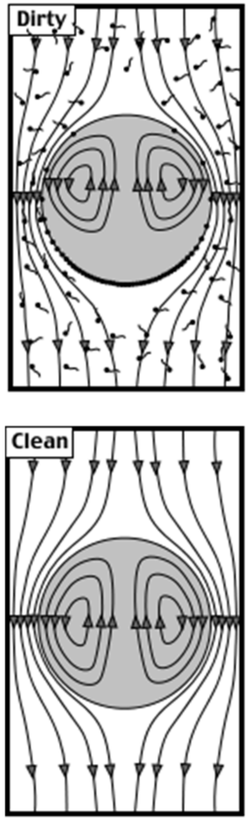
$$C_D(Re_p) = \begin{cases} \dfrac{24}{Re_p}\left(1 + 0.15 Re_p^{0.687}\right) & \text{for} \quad Re_p < 1000 \\ 0.44 & \text{for} \quad 1000 < Re_p < 3 \times 10^6 \end{cases}$$

$$Re_p = \rho_1 d_{eq} \left|\mathbf{U}_{rel}\right| / \mu_1$$

Drag coefficient for a bubble/drop

Fig. from Clift, Grace & Weber 1978





Reduced drag due to internal circulation

Further hydrodynamic forces

- Virtual (added) mass force
  - Sphere: $C_{\mathrm{vm}} = 0.5$

$$\mathbf{F}_{\mathrm{VM}} = C_{\mathrm{VM}} \mathcal{V}_{\mathrm{p}} \rho_1 \frac{\mathrm{d}\mathbf{U}_{\mathrm{rel}}}{\mathrm{d}t}$$

Acceleration/deceleration

- Transversal lift force
  - Particle rotation
  - Particle in shear flow

$$\mathbf{F}_{\mathrm{L}} = C_{\mathrm{L}} \mathcal{V}_{\mathrm{p}} \rho_1 \mathbf{U}_{\mathrm{rel}} \times \left(\nabla \times \mathbf{v}_{\mathrm{liquid}} \right)$$

- History force (is usually neglected)
- Turbulent dispersion force, e.g. $\mathbf{F}_{\mathrm{TD}} = -C_{\mathrm{TD}} \mathcal{V}_{\mathrm{p}} \rho_1 k_1 \nabla \alpha_1$
- Wall lubrication force

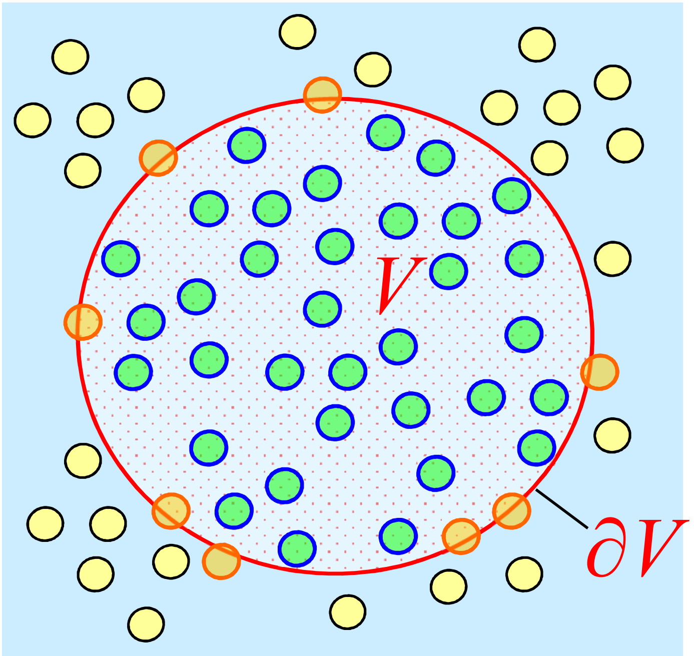
(k_1 = liquid turbulent kinetic energy)

- …

For a comparison of 14 different formulations for the drag coefficient and of 8 for the lift coefficient see Pang & Wei *Nucl Eng Des* **241** (2011) 2204

Closure of the two-fluid model (1)

<u>Assumption:</u> the volume of the particles is much smaller than that of the mesh cell, i.e. $\mathcal{V}_\mathrm{p} \ll V$



$$\mathbf{M}_{1,\mathrm{h}} = -\frac{1}{V}\iint_{\Gamma\cap V}\left(-p_{1,\mathrm{dyn}}\mathbb{I} + 2\mu_1\mathbb{D}_1\right)\cdot\hat{\mathbf{n}}_\Gamma \mathrm{d}s$$

$$\approx -\frac{1}{V}\sum_{j=1}^{N_\mathrm{p}}\oiint_{\mathcal{A}_\mathrm{p}^j}\left(-p_{1,\mathrm{dyn}}\mathbb{I} + 2\mu_1\mathbb{D}_1\right)\cdot\hat{\mathbf{n}}_\Gamma \mathrm{d}s$$

$$= -\frac{1}{V}\sum_{j=1}^{N_\mathrm{p}}\mathbf{F}_\mathrm{hydr}^j$$

N_p = number of particles in V

Dynamic boundary condition:

$$\mathbf{M}_{1,\mathrm{h}} + \mathbf{M}_{2,\mathrm{h}} = \frac{1}{V}\iint_{\Gamma\cap V} 2\sigma H\hat{\mathbf{n}}_\Gamma \mathrm{d}s$$

$$\approx \frac{1}{V}\sum_{j=1}^{N_\mathrm{p}}\oiint_{\mathcal{A}_\mathrm{p}^j} 2\sigma H\hat{\mathbf{n}}_\Gamma \mathrm{d}s = 0$$

Closure of the two-fluid model (2)

Assumption: the flow is mono-disperse so that all particles have the same volume $\mathcal{V}_\mathrm{p} = \pi d_\mathrm{eq}^3 / 6$

$$\mathbf{M}_{1,\mathrm{h}} \approx -\frac{1}{V}\sum_{j=1}^{N_\mathrm{p}} \mathbf{F}_\mathrm{hydr}^j \approx -\underbrace{\frac{N_\mathrm{p}}{V}}_{=n_\mathrm{p}} \mathbf{F}_\mathrm{hydr} = -\underbrace{\frac{N_\mathrm{p}\mathcal{V}_\mathrm{p}}{V}}_{=\alpha_2} \frac{1}{\mathcal{V}_\mathrm{p}} \left(\mathbf{F}_\mathrm{drag} + \mathbf{F}_\mathrm{vm} + \mathbf{F}_\mathrm{lift} + \mathbf{F}_\mathrm{hist} + \ldots \right)$$

$$\mathbf{M}_{1,\mathrm{drag}} = -\frac{\alpha_2}{\mathcal{V}_\mathrm{p}} \mathbf{F}_\mathrm{drag} = \frac{1}{2} \frac{A_\mathrm{p}}{\mathcal{V}_\mathrm{p}} C_\mathrm{D} \alpha_2 \rho_1 \mathbf{U}_\mathrm{rel} \left| \mathbf{U}_\mathrm{rel} \right|$$

$$\mathbf{U}_\mathrm{rel} = \overline{\mathbf{v}_2}^2 - \overline{\mathbf{v}_1}^1$$

From solution of the two momentum eqs

$$\frac{A_\mathrm{p}}{\mathcal{V}_\mathrm{p}} \approx \frac{\pi d_\mathrm{eq}^2 / 4}{\pi d_\mathrm{eq}^3 / 6} = \frac{3}{2} \frac{1}{d_\mathrm{eq}}$$

Equivalent bubble diameter d_eq must be specified!

Closure of the two-fluid model (3)

- Heat transfer across the interface

$$q_{k,\mathrm{i}} = Q_{k,\mathrm{i}} / A_\mathrm{i} = h_{k,\mathrm{i}} (\overline{T_k}^{k} - T_\mathrm{i}) \qquad q_{1,\mathrm{i}} + q_{2,\mathrm{i}} = 0$$

- Phase change (boiling/condensation)

$$T_\mathrm{i} = T_\mathrm{sat} \qquad q_{1,\mathrm{i}} + q_{2,\mathrm{i}} = \dot{m}(h_2^\mathrm{sat} - h_1^\mathrm{sat})$$

- Interfacial heat transfer coefficient $h_{1,\mathrm{i}}$
  - Ranz-Marshall correlation ($0 < Re_\mathrm{p} < 200;\ 0 < Pr_1 < 250$)

$$Nu \equiv \frac{h_{1,\mathrm{i}} d_\mathrm{p}}{\lambda_1} = 2 + 0.6 Re_\mathrm{p}^{0.5} Pr_1^{0.33} \qquad Pr_1 = \frac{\mu_1 c_{\mathrm{p},1}}{\lambda_1}$$

Ranz & Marshall *Chem Eng Prog* **48** (1952) 141

Example for application of the TFM: mixing in a bubble plume

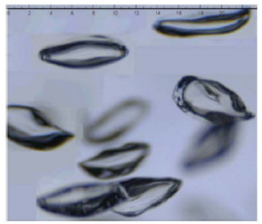
Background:

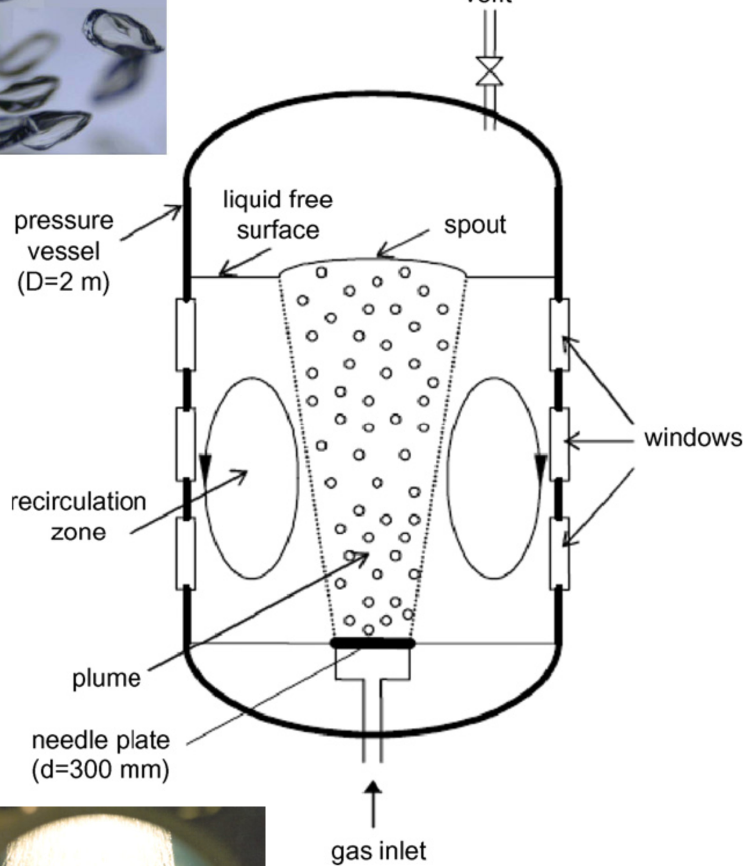
Pressurized Thermal Shock (PTS) in a PWR

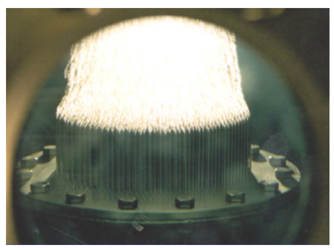
- Fast temperature or pressure transients yield non-uniform temperature distribution and induce stresses in the pressure vessel wall
- Irradiation reduces ductility of pressure vessel wall and makes reactor more prone for cracks and failure
- A key phenomenon during the PTS events is the bubble-induced mixing (was one of the topics in the EU project NURESIM)

Bubble plume experiment

- LINX facility at PSI (CH)
  - Cylindrical vessel
    (2 m diameter, 3.4 m height)
- Turbulent bubble plume
  - Needle plate: 350 capillaries
  - Bubble diameter 2-3 mm
- Measurements
  - Time-averaged radial void fraction profiles (opt. probes)
  - Instantaneous bubble and liquid velocity distributions (particle image velocimetry)





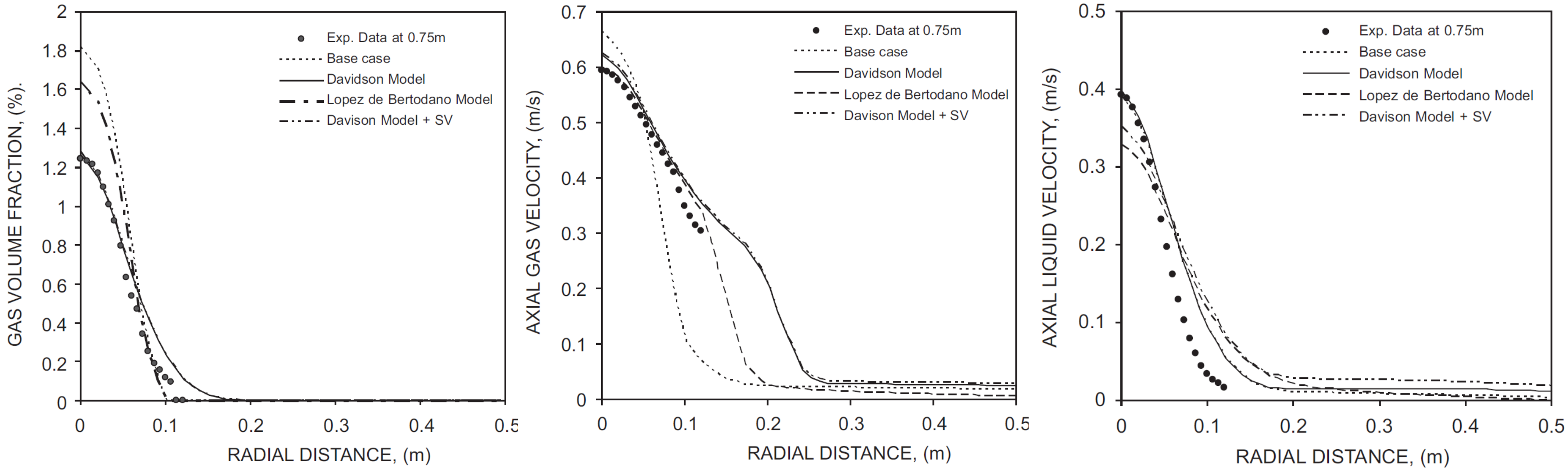


Computations with two-fluid model*

- Code CFX 4.3
- Modeled hydrodynamic forces
  - Drag force (influence of C_{D}, four different models)
  - Virtual mass force (standard formulation with $C_{\mathrm{vm}} = 0.5$)
  - Lift force (standard formulation with $C_{\mathrm{L}} = 0.1$)
  - Turbulent dispersion force (two different formulations)
- Turbulence model (for liquid phase only)
  - k-ε model of Launder & Spalding with standard coeff.
  - Term in k- and ε-eq. for bubble-induced turbulence (BIT)

* Dhotre & Smith *Chem Eng Sci* **62** (2007) 6615

Comparison experiment-simulation (1)



– “Base case” (BC): $C_D = 0.44$, $C_L = 0.1$, no TD

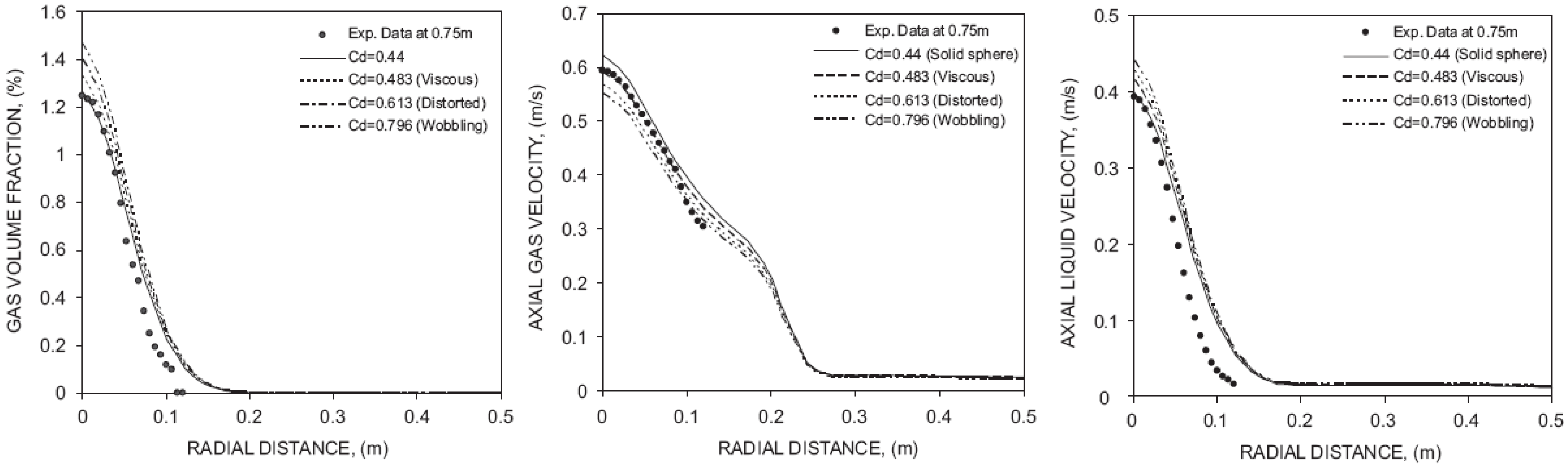
– “Davidson model“: BC + TD model of Davidson

– „Lopez de Bertodano model“: BC + TD model of Lopez de Bertodano

– „Davidson model + SV“: BC + TD model of Davidson + BIT model of Simonin & Viollet

gives best agreement

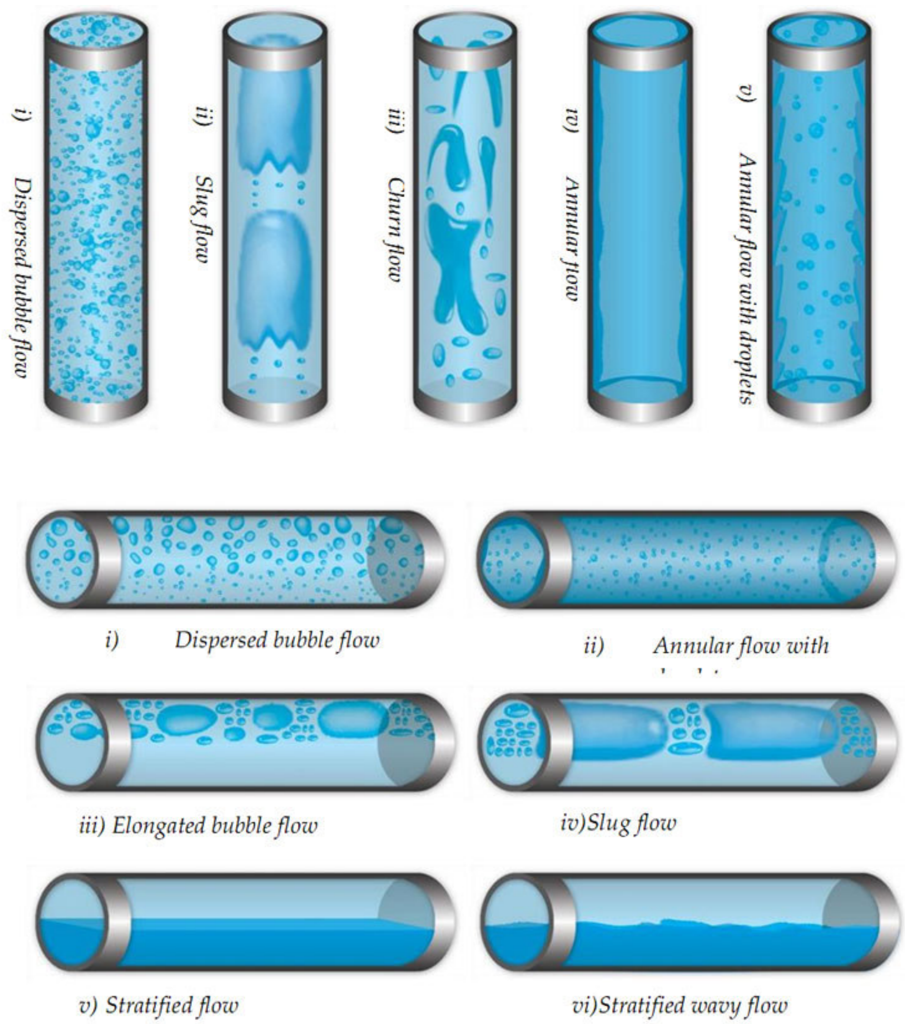
Comparison experiment-simulation (2)



- BC + TD model of Davidson + BIT model of Simonin & Viollet and **variation of drag coefficient** ($C_D = 0.44$ gives best results)
- Predictions of void fraction, axial gas and liquid velocity are in reasonable agreement with exp. data except close to the injector
- Poor agreement for turb. kinetic energy and turb. shear stresses

Closure laws for other flow regimes

- Interfacial exchange of momentum and energy depend strongly on the flow regime
- Closure relations for wavy/annular/slug/churn flow have been mainly developed for the *one-dimensional* two-fluid model



Limitations of the standard TFM

- The flow regime must be known in advance in order to specify meaningful models for the interfacial transfer of momentum/heat
- Limitations for disperse flow regime
  - only mono-disperse flow (bubble diameter is “input”)
  - coalescence/ breakup result in bubble size distribution
  - hydrodynamic forces depend on bubble size/volume
- Extension of standard TFM must account for a *variable* bubble size or interfacial length scale

Extensions of the standard TFM

- Four-field two fluid-model
  - Continuous liquid, disperse liquid, continuous vapor, disperse vapor
  - see e.g. R. Lahey, *Nucl Eng Des* **235** (2005) 1043

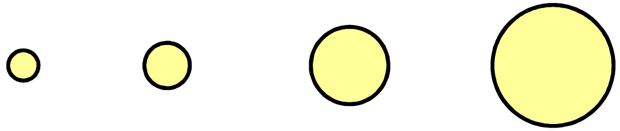
Twelve equations:
mass, momentum & energy for each of the four fields

- Multi-size group models
  - Suitable for disperse flows only
- Interfacial area transport equation (IATE)
  - Suitable for all flow regimes

see next two pages

Multi-size group (MUSIG) models

- Size distribution is represented by M groups/classes



$$\mathcal{V}_{p,1} < \mathcal{V}_{p,2} < \ldots \mathcal{V}_{p,k} \cdots < \mathcal{V}_{p,M}$$

$$\mathbf{M}_1 \approx -\sum_{k=1}^{M} \underbrace{\frac{\alpha_{2,k}}{\mathcal{V}_{p,k}}}_{=n_{p,k}} \mathbf{F}_{\text{hydr},k} \qquad \alpha_2 = \sum_{k=1}^{M} \alpha_{2,k}$$

- Multi-field formulation for poly-disperse flows
  - 1 mass and 1 momentum conservation eq for liquid phase
  - M mass conservation eqs for gas phase

$$\frac{\partial \alpha_{2,k}\rho_2}{\partial t} + \nabla \cdot (\alpha_2 \rho_2 \overline{\mathbf{v}_{2,k}}^2) = S_k$$

Source term due coalescence/break-up

  - $N \leq M$ momentum cons. eqs for gas phase (some groups share a velocity field)
  - CPU time increases with M and N

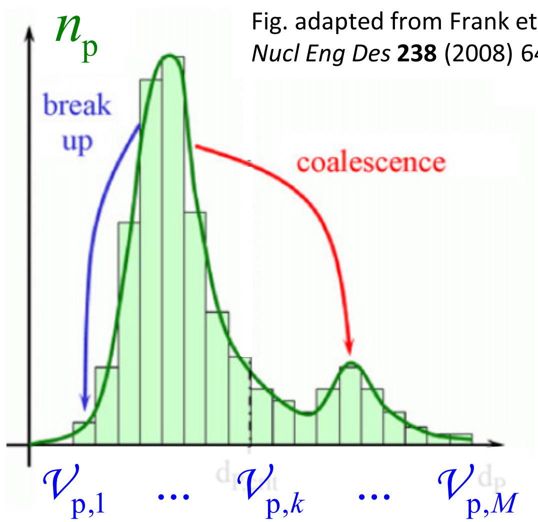


Fig. adapted from Frank et al. *Nucl Eng Des* **238** (2008) 647

Interfacial area transport eq (IATE)

- Interfacial area concentration

  $a_i \equiv A_i / V \quad [1/\mathrm{m}]$ (inverse of a length scale)

- Transport equation for a_i

$$\frac{\partial a_i}{\partial t} + \nabla \cdot (a_i \mathbf{v}_i) = S_{\text{Breakup}} - S_{\text{Coalescence}} \pm S_{\text{Expansion/Contraction}} \pm S_{\text{Boiling/Condensation}}$$

Modeling of source/sink terms is a challenge

- Ishii & Hibiki: 1D two-group IATE
  - Gr. 1: spherical and ellipsoidal bubbles
  - Gr. 2: cap-type and elongated bubbles

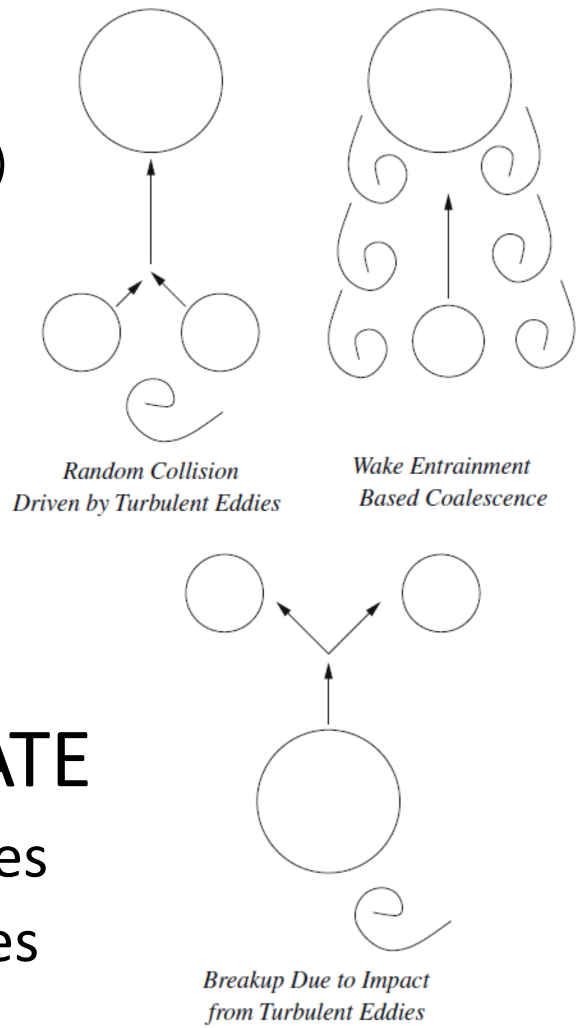


Fig. from Vasavasa et al. *Int J Multiph Flow* **35** (2009) 323

Content

- Introduction
  - CFD in nuclear engineering
  - Gas-liquid two phase flows
- Governing equations
  - Local equations
  - Averaging and closure problem
- Models for interpenetrating continua
  - Homogeneous model
  - Algebraic slip model and drift-flux model
  - Two-fluid model and its advanced variants
- **Final remarks**

Scientific challenges for CMFD

- Polydisperse flows
  - Kernel functions for probabilities of coalescence/breakup
- 3D closure relations for non-disperse flow regimes
  - E.g. churn-turbulent flow
- Transition between different flow regimes
- Turbulence modeling (interface-turbulence interactions)
  - Statistical models (Reynolds averaged Navier-Stokes eqs)
  - Large eddy simulation techniques for flows with interfaces
    - Filtering of velocity field and interface (D. Lakehal; O. Lebaigue)
  - Wall functions
- Multi-scale models and hybrid models
- …

Best practice guidelines

- F. Menter
  CFD Best Practice Guidelines for CFD Code Validation for Reactor Safety Applications
  EC Project ECORA, Report EVOL-ECORA-D 01, Feb. 2002
  (https://domino.grs.de/ecora/ecora.nsf)
- M. Casey, T. Wintergerste
  Best practice guidelines for industrial computational fluid dynamics of single-phase flows
  ERCOFTAC 2002
- M. Sommerfeld, B. van Wachem, R. Oliemans
  Best practice guidelines for computational fluid dynamics of dispersed multiphase flows
  ERCOFTAC 2008

Topical NED issues related to CFD

Nuclear Engineering and Design

Volume 238, Issue 3, Pages 443-786 (March 2008)

Benchmarking of CFD Codes for Application to Nuclear Reactor Safety
Munich, Germany
05-07 September 2006
Edited by Brian L. Smith and Yassin Hassan

Nuclear Engineering and Design

Volume 240, Issue 9, Pages 2075-2382 (September 2010)

Experiments and CFD Code Applications to Nuclear Reactor Safety (XCFD4NRS)
Edited by Brian L. Smith, Dominique Bestion and Yassin Hassan