Multiphase and Reactive Flow Modelling

BMEGEÁT(MW17|MG27)

Part 2

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Phases

! Incomplete without class notes

Mathematical description

using <u>characteristic functions:</u>

$$\chi^{(p)}(t,\vec{\mathbf{r}}) = \begin{cases} 1 & \text{if } \vec{\mathbf{r}} \text{ is in phase } p \text{ at time } t, \\ 0 & \text{if } \vec{\mathbf{r}} \text{ is in another phase at time } t. \end{cases}$$

They resemble concentrations since one of them is redundant:

$$\sum_p \chi^{(p)}(t,\vec{\mathbf{r}}) = 1$$

but they are discreet and not continuous (either 0 or 1, but not in between)

Interfaces

Incomplete without class notes

- Mathematical description of interfaces
  - normal, tangent, curvature
  - implicit description
  - parametric description
  - interface motion
- Transport through interfaces

  Continuity and jump conditions:
  - mass balance
  - force balance
  - heat balance

Interfaces and their motion

- Description of interface surfaces:
  - parametrically
  - by implicit function
  - (the explicit description is the common case of the previous two)

New primary(?) field variables

- Moving phase interface:
  (only!) the normal velocity component makes sense

!

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Description of an interface by an implicit function

$$F(t,x,y,z)=0$$

$$\mathbf{n}=\nabla F/|\nabla F| \ \text{(unit normal)}$$

$$\kappa=\frac{1}{2}\cdot\left(\frac{1}{R_1}+\frac{1}{R_2}\right)=\nabla\cdot\mathbf{n} \ \text{(mean curvature)}$$

TypeI surface integrals $\leftrightarrow$ volume integrals :

$$\iint f(t,x,y,z)\cdot dA=\iiint f(t,x,y,z)\cdot\delta\big(F(t,x,y,z)\big)\cdot|\nabla F(t,x,y,z)|\cdot dV$$

TypeII surface integrals $\leftrightarrow$ volume integrals :

$$\iint \mathbf{v}(t,x,y,z)\cdot\mathbf{dA}=\iiint \mathbf{v}(t,x,y,z)\cdot\delta\big(F(t,x,y,z)\big)\cdot\nabla F(t,x,y,z)\cdot dV$$

Equation of motion of an interface given by implicit function

- Equation of interface

$$F(t,\mathbf{r}) = 0$$

- Path of the point that remains on the interface (but not necessarily a fluid particle)

$$\mathbf{r}(t)$$

$$F(t,\mathbf{r}(t)) = 0$$

- Differentiate

$$\frac{d}{dt}F(t,\mathbf{r}(t)) = \partial_t F + \dot{\mathbf{r}}(t)\cdot\nabla F = 0$$

$$\updownarrow$$

- For any such point the normal velocity component must be the same

$$\partial_t F + u_\perp^* \cdot \mathbf{n}\cdot\nabla F = 0$$

$$u_\perp^* = \mathbf{n}\cdot\dot{\mathbf{r}}(t)$$

- Propagation speed and velocity of the interface

$$\mathbf{u}_\perp^* = \mathbf{n}\cdot u_\perp^*$$

Only the normal component makes sense

Parametric description of interface motion

- Functional form of the surface: $\mathbf{r}(t,a,b)$
- Curvilinear coordinates and $a(t), b(t)$
- path of a point that remains on the interface $\mathbf{r}(t,a(t),b(t))$
  (not necessarily a fluid particle)
- Differentiate:

$$\frac{d}{dt}\mathbf{r}(t,a(t),b(t)) =$$

$$= \partial_t \mathbf{r} + \partial_a \mathbf{r} \cdot \dot{a}(t) + \partial_b \mathbf{r} \cdot \dot{a}(t)$$

- Take the normal velocity component to get

$$\mathbf{n} = \frac{\partial_a \mathbf{r} \times \partial_b \mathbf{r}}{\left|\partial_a \mathbf{r} \times \partial_b \mathbf{r}\right|}$$

- the propagation speed and velocity of the interface:

$$u_\perp^* = \mathbf{n} \cdot \dot{\mathbf{r}}(t) = \mathbf{n} \cdot \partial_t \mathbf{r}(t,a(t),b(t))$$

$$\mathbf{u}_\perp^* = \mathbf{n} \cdot u_\perp^*$$

Mass balance through an interface

Steps of the derivation:

1. Describe in a reference frame that moves with the interface (e.g. keep the position of the origin on the interface)
2. Describe velocities inside the phases in the moving frame
3. Match mass fluxes

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The kinematical boundary conditions

The net mass flux through the interface :

$$j^{*}_{\text{mass}} \overset{\text{def}}{=} \rho^{(1)}\left(\mathbf{u}^{(1)} - \mathbf{u}^{*}_{\perp}\right)\cdot\mathbf{n} \equiv \rho^{(2)}\left(\mathbf{u}^{(2)} - \mathbf{u}^{*}_{\perp}\right)\cdot\mathbf{n}$$

$$\left[\rho\left(\mathbf{u} - \mathbf{u}^{*}_{\perp}\right)\cdot\mathbf{n}\right] = 0$$

For the tangential components:

$$[\mathbf{u}\times\mathbf{n}] = \mathbf{0} \ \text{(no slip condition)}$$

This condition does not follow from mass conservation

$$\partial_t F + \mathbf{u}^{*}_{\perp}\cdot\nabla F = 0$$

!

Incomplete without class notes

Without (net) mass transfer:

$$j^{*}_{\text{mass}} = 0 \Rightarrow \mathbf{u}^{(1)}\cdot\mathbf{n} = \mathbf{u}^{(2)}\cdot\mathbf{n} = \mathbf{u}^{*}_{\perp}\cdot\mathbf{n} \equiv u^{*}_{\perp}$$

$$[\mathbf{u}\cdot\mathbf{n}] = 0$$

tangential components:

$$[\mathbf{u}\times\mathbf{n}] = \mathbf{0}$$

$$\Rightarrow [\mathbf{u}] = \mathbf{0}$$

continuity of velocity

$$\partial_t F + \mathbf{u}\cdot\nabla F = 0$$

conservation of interface

Diffusion through an interface

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Mass flux of component k in the co-moving reference frame:

$$\rho_k\left(\mathbf{u}_k - \mathbf{u}_\perp^*\right) = c_k\rho\left(\mathbf{u} - \mathbf{u}_\perp^* + \mathbf{u}_k - \mathbf{u}\right) = c_k\rho\left(\mathbf{u} - \mathbf{u}_\perp^*\right) + \mathbf{j}_k$$

Case of conservation of component mass:

- on a pure interface (no surface phase, no surfactants)
- without surface reactions (not a reaction front)

$$\Rightarrow \begin{cases} \left[\rho_k\left(\mathbf{u}_k - \mathbf{u}_\perp^*\right)\cdot\mathbf{n}\right] = 0 \\ \Updownarrow \\ \left[c_k\right]\cdot j^*_{\text{mass}} + \left[\mathbf{j}_k\cdot\mathbf{n}\right] = 0 \end{cases}$$

The component flux through the interface:

$$j_k^* \overset{\text{def}}{=} \rho_k^{(1)}\left(\mathbf{u}_k^{(1)} - \mathbf{u}_\perp^*\right)\cdot\mathbf{n} \equiv \rho_k^{(2)}\left(\mathbf{u}_k^{(2)} - \mathbf{u}_\perp^*\right)\cdot\mathbf{n}$$

$$= c_k^{(1)}\cdot j^*_{\text{mass}} + \mathbf{j}_k^{(1)}\cdot\mathbf{n} \equiv c_k^{(2)}\cdot j^*_{\text{mass}} + \mathbf{j}_k^{(2)}\cdot\mathbf{n}$$

Examples

Impermeability condition

Surface reaction

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Momentum balance through an interface

Effects due to

- surface tension (S)
- surface viscosity
- surface compressibility
- mass transfer

Dynamical boundary conditions with surface/interfacial tension

- Fluids in rest
  - normal component: $\left[p\right] = 2\,S\,\kappa$

Modifies the thermodynamic phase equilibrium conditions

- Moving fluids without interfacial mass transfer
  - normal component: $\left[p - \mathbf{n}\cdot\left(\boldsymbol{\tau}\,\mathbf{n}\right)\right] = 2\,S\,\kappa$
  - tangential components: $\left[-\,\mathbf{t}\cdot\left(\boldsymbol{\tau}\,\mathbf{n}\right)\right] = \mathbf{t}\cdot\nabla S \quad \left(\mathbf{t}\perp\mathbf{n}\right)$

The viscous stress tensor: $\tau_{ij} = \mu\cdot\left(\partial_i u_j + \partial_j u_i\right)$

!

Incomplete without class notes

The heat conduction equation

Transport equation in the bulk

- Fourier's formula
  - (thermodiffusion not included!)
- Volumetric heat sources:
  - viscous dissipation
  - direct heating
  - heat released in chemical reactions

$$\rho c_p \left(\partial_t T + \mathbf{u} \cdot \nabla T \right) = -\nabla \mathbf{j}_{\text{heat}} + \dot{q}_{\text{heat}}$$

$$\mathbf{j}_{\text{heat}} = -\lambda \cdot \nabla T$$

Conditions on the interfaces

- Thermal equilibrium
- Heat flux:
  - continuity (simplest)
  - latent heat (phase transition of pure substance)

  Even more complex cases:
  - chemical component diffusion
  - chemical reactions on surface
  - direct heating of surface

$$\left[T \right] = 0$$

$$\left[\mathbf{n} \cdot \mathbf{j}_{\text{heat}} \right] = 0$$

$$\left[\mathbf{n} \cdot \mathbf{j}_{\text{heat}} \right] = L \cdot j^*_{\text{mass}}$$

$$\left[\mathbf{n} \cdot \mathbf{j}_{\text{heat}} \right] = \ldots$$

Jump conditions

Summary of boundary conditions on moving interfaces

Physical balance equations imply conditions on the interface elements:

- continuity conditions
- jump conditions

These are different

- with and without mass transfer
- in case of special interfacial properties (`active interfaces')

Classification of multiphase models

`Fine´ models

(single fluid models)

- The position of the moving interfaces are described in the model

`Rough´ models

(interpenetrating media models)

- The position of the interfaces are not described in the model

1. *n*-fluid (e.g two-fluid) models
   - The phase transfer processes are modelled explicitly

2. mixture models
   - The phase transfer processes are parametrised in the constitutive equations rather than being modelled explicitly

Approaches of fine models

Phase-by-phase

- Separate sets of governing equations for the domains of each phase
- Each phase is treated as a simple fluid
- Describing/capturing moving interfaces
- Prescribing jump conditions at the interfaces

One-fluid

- A single set of governing equation covering the domains of all phases
- Complicated constitutional equations
- Describing/capturing moving interfaces
- Jumps on the interfaces are described as singular source terms in the governing equations

Phase-by-phase mathematical models

1. A separate phase domain for each phase
2. A separate set of balance equations for each phase domain, for the primary field variables introduced for the single phase problems, supplemented by the constitutional relations describing the material properties of the given phase
3. The sub-model for the motion of phase domains and phase boundaries (further primary model variables)
4. Prescribing the moving boundary conditions: coupling among the field variables of the neighbouring phase domains and the interface variables (via jump conditions)

$p^{(p)}(t,\vec{\mathbf{r}}),\ \vec{\mathbf{u}}^{(p)}(t,\vec{\mathbf{r}}),\ T^{(p)}(t,\vec{\mathbf{r}}),\ldots$

$\rho^{(p)}(T,p,\ldots),\ \mu^{(p)}(T,p,\ldots),\ k^{(p)}(T,p,\ldots),\ldots$

e.g. $F(t,\vec{\mathbf{r}})=0$

The one-fluid mathematical model

1. A single fluid domain
2. Characteristic function for each phase
3. Material properties expressed by the properties of individual phases and the characteristic functions
4. A single set of balance equations for the primary field variables introduced for the single phase problems, supplemented by discrete source terms describing interface processes
5. The sub-model for the motion of phase domains and phase boundaries (further primary model variables)

$$\chi^{(p)}(t,\vec{\mathbf{r}}) = 1 \text{ or } 0$$

$$\sum_p \chi^{(p)}(t,\vec{\mathbf{r}}) = 1$$

$$\rho = \sum_p \chi^{(p)} \cdot \rho^{(p)}$$

$$\mu = \sum_p \chi^{(p)} \cdot \mu^{(p)}$$

$$k = \sum_p \chi^{(p)} \cdot k^{(p)}$$

$$p(t,\vec{\mathbf{r}}),\ \vec{\mathbf{u}}(t,\vec{\mathbf{r}}),\ T(t,\vec{\mathbf{r}}),\ldots$$

$$\chi^{(p)}(t,\vec{\mathbf{r}}) \text{ or something equivalent}$$

The sub-models of phase motion (interface sub-models)

- The choice of the mathematical level sub-model is influenced by the available effective numerical methods.

Numerical implementations of interface sub-models

Main categories

- Grid manipulation
- Front capturing: implicit interface representation
- Front-tracking: parametric interface representation
- Full Lagrangian

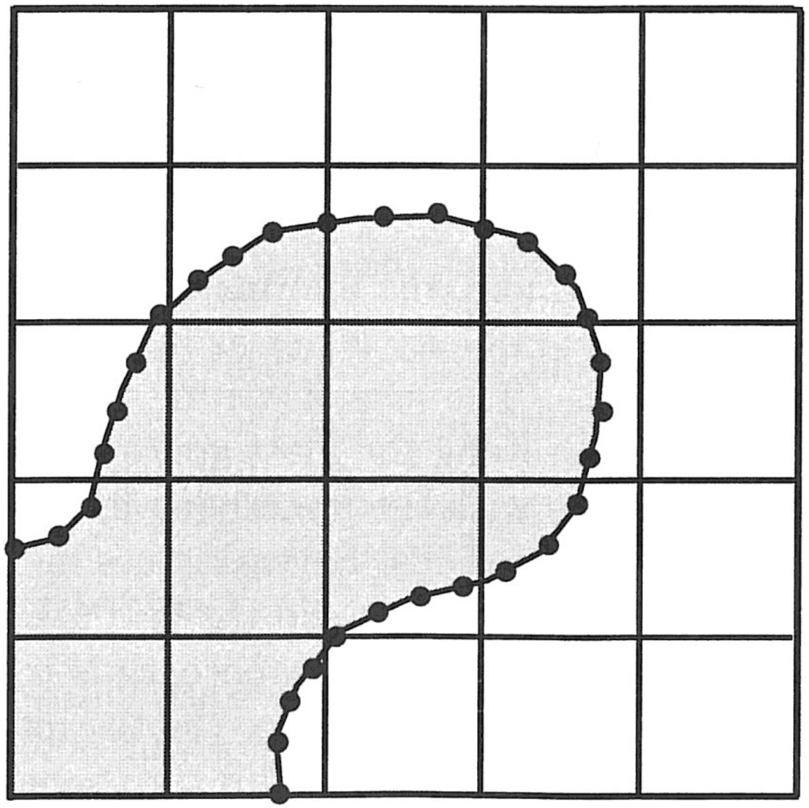
Specific methods

- MAC: (Marker-And-Cell)
- VOF: (Volume-of-Fluid)
- level-set
- phase-field
- CIP

E.g. SPH

Front tracking methods

on a fixed grid
by connected *marker points*



(Suits the parametric mathematical description)

- In 3D: triangulated unstructured grid represents the surface

Tasks to solve:

- Advecting the front
- Interaction with the grid (efficient data structures are needed!)
- Merging and splitting (hard!)

MAC
(Marker-And-Cell method)

- An interface reconstruction — front capturing — model (the primary variable is the characteristic function of the phase domain, the interface is reconstructed from this information)
- The naive numerical implementation of the mathematical transport equation $\partial_t \chi + \nabla(\chi \cdot u) = 0$:
  - 1st (later 2nd) order upwind differential scheme
- Errors (characteristic to other methods as well!):
  - numerical diffusion in the 1st order
  - numerical oscillation in higher orders

Due to the discontinuities of the function

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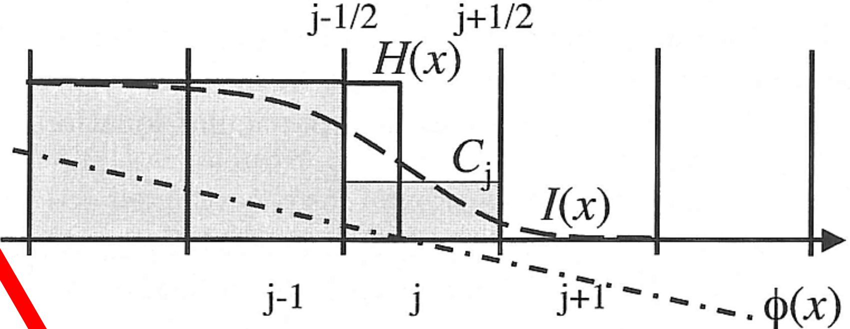
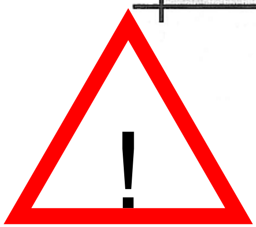
MAC





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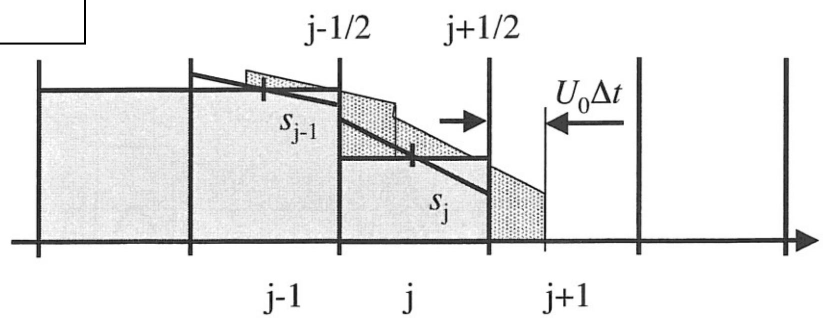
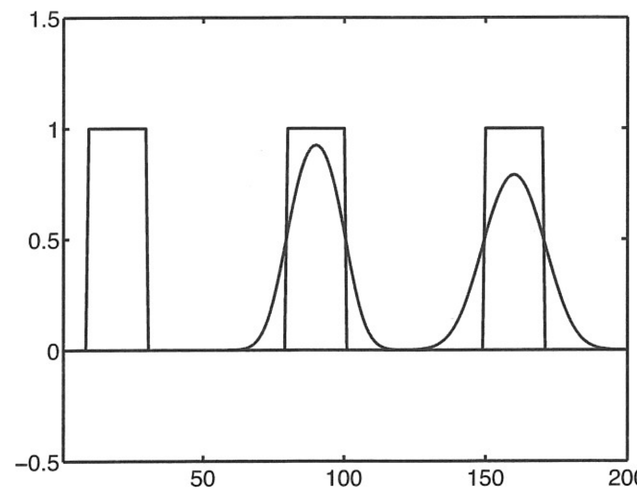
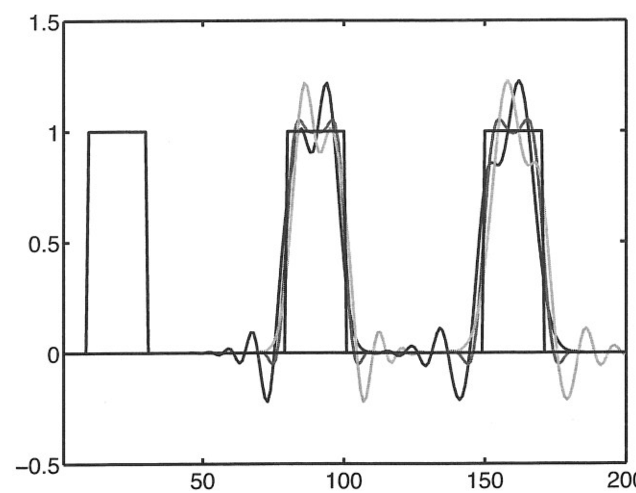
$$C_j^{n+1} = C_j^n - \frac{u \cdot \Delta t}{h} \cdot \left(C_j^n - C_{j-1}^n \right)$$





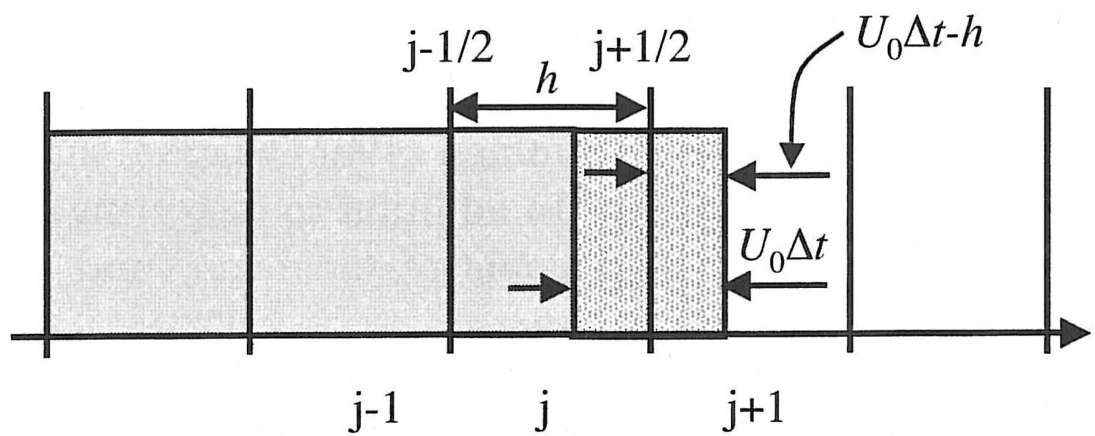


VOF
(Volume-Of-Fluid method)

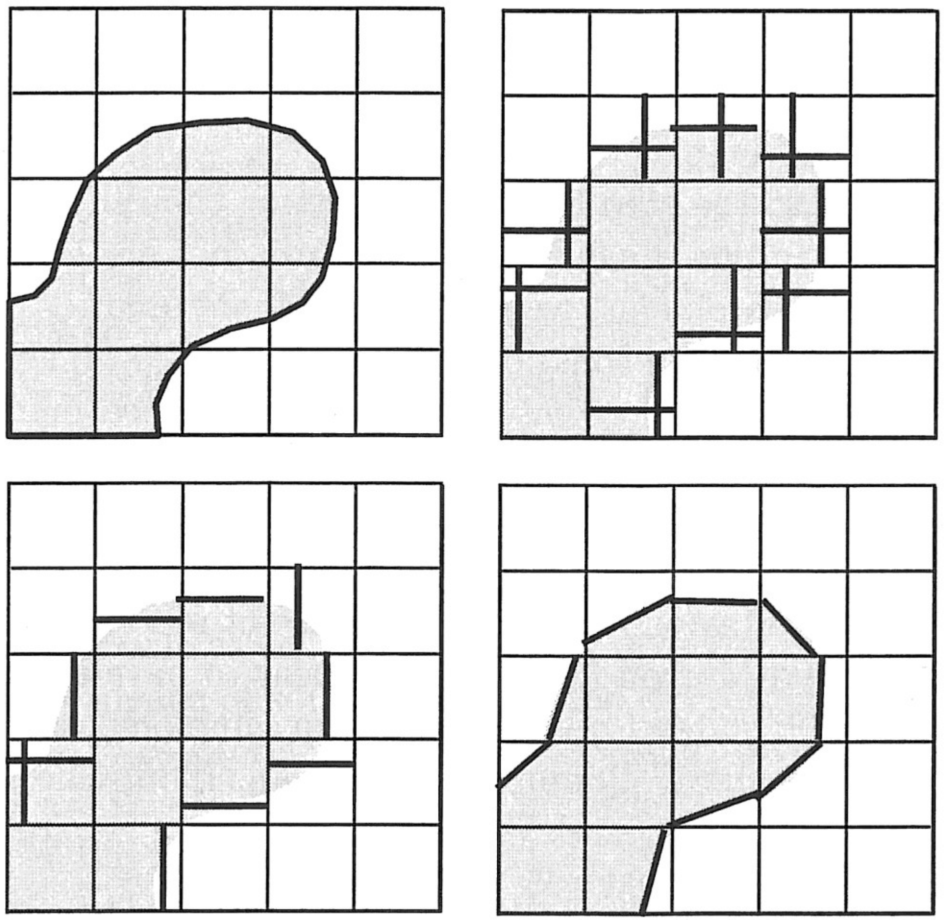
1D version (1st order explicit in time):

- Gives a sharp interface, conserves mass
- Requires special algorithmic handling

The scheme of evolution:



VOF in 2D and 3D



SLIC:
Simple Line
Interface Construction

PLIC:
Piecewise Linear
Interface Construction

Hirt & Nichols

ANSYS FLUENT

ANSYS FLUENT

Numerical steps of VOF

1. Interface reconstruction within the cell
   1. determine **n**
      - several schemes
   2. position straight interface
2. Interface advection
   - several schemes exist, competing goals:
     - conserve mass exactly
     - avoid diffusion
     - avoid oscillations
3. Compute the surface tension force in the Navier–Stokes eqs.
   - several schemes

Why are so many possible schemes?
Information based on the cell and neighbour values are redundant (overdetermined)

Implementation of VOF in ANSYS FLUENT

- Any number of phases can be present
- The transport equation for is adapted to allow
  - variable density of phases
  - mass transport between phases
- Contact angle model at solid walls is coupled
- Special (`open channel´) boundary conditions for VOF
- Surface tension is implemented as a *continuous surface force* in the momentum equation

- For the flux calculations ANSYS FLUENT can use one of the following schemes:
  - Geometric Reconstruction: PLIC, adapted to non-structured grids
  - Donor-Acceptor: Hirt & Nichols, for quadrilateral or hexahedral grid only
  - Compressive Interface Capturing Scheme for Arbitrary Meshes (CICSAM): a general purpose sheme for sharp jumps (e.g. high ratios of viscosities) for arbitrary meshes
  - Any of its standard schemes (probably diffuse and oscillate)

The level set method [hu: nívófelület-módszer]

$$F(t,x,y,z)=0$$

$$\mathbf{n}=\nabla F/|\nabla F|$$

$$\partial_t F + u_\perp^* \cdot \mathbf{n} \cdot \nabla F = 0$$

$$\kappa = \frac{1}{2}\cdot\left(\frac{1}{R_1}+\frac{1}{R_2}\right)=\nabla\cdot\mathbf{n}$$

$$\iint f(t,x,y,z)\cdot dA = \iiint f(t,x,y,z)\cdot\delta(F(t,x,y,z))\cdot|\nabla F(t,x,y,z)|\cdot dV$$

$$\iint \mathbf{v}(t,x,y,z)\cdot \mathbf{dA} = \iiint \mathbf{v}(t,x,y,z)\cdot\delta(F(t,x,y,z))\cdot\nabla F(t,x,y,z)\cdot dV$$

$$\iiint 2S\kappa\cdot\delta(F(\ldots))\cdot\nabla F\cdot dV$$

- the interface is implicit
- *F* is continuous
  - **standard advection schemes work fine**
- the curvature can be obtained easily
- the effect of surface tension within a cell can be computed

The level set method

$$F(t,x,y,z)=0$$

$$\mathbf{n}=\nabla F$$

$$\partial_t F + u_\perp^* = 0$$

$$\kappa = \frac{1}{2}\cdot\left(\frac{1}{R_1}+\frac{1}{R_2}\right) = \nabla\cdot\mathbf{n} = \nabla^2 F$$

$$\iint f(t,x,y,z)\cdot dA = \iiint f(t,x,y,z)\cdot\delta(F(t,x,y,z))\cdot dV$$

$$\iint \mathbf{v}(t,x,y,z)\cdot\mathbf{dA} = \iiint \mathbf{v}(t,x,y,z)\cdot\delta(F(t,x,y,z))\cdot\nabla F(t,x,y,z)\cdot dV$$

$$\iiint 2S\kappa\cdot\delta(F(\ldots))\cdot\nabla F\cdot dV$$

- If $|\nabla F(t,x,y,z)|=1$ then the computational demand can be substantially decreased

Signed distance function as an implicit level-set function

$$F(t,x,y,z)=0,\ \left|\nabla F(t,x,y,z)\right|=1$$

$$\partial_t F + \mathbf{u}_\perp^* \cdot \nabla F = 0$$

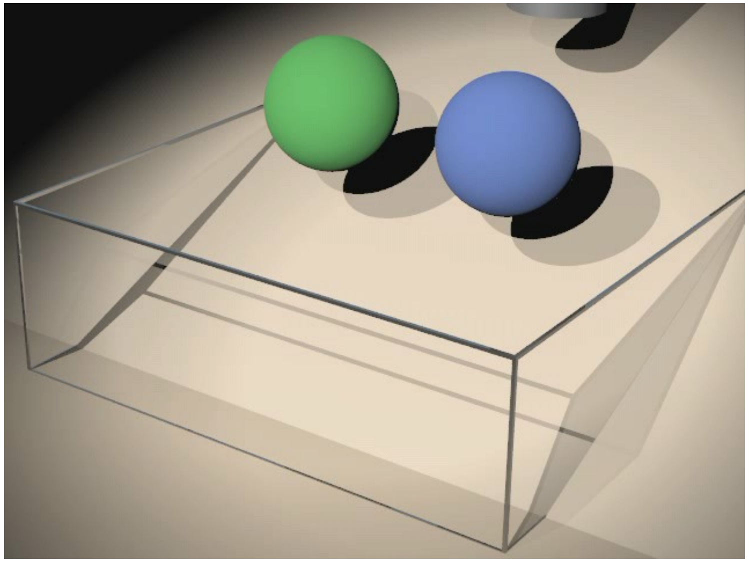
$$\partial_\tau F + S(F)\cdot\left(\left|\nabla F\right|-1\right)=0$$

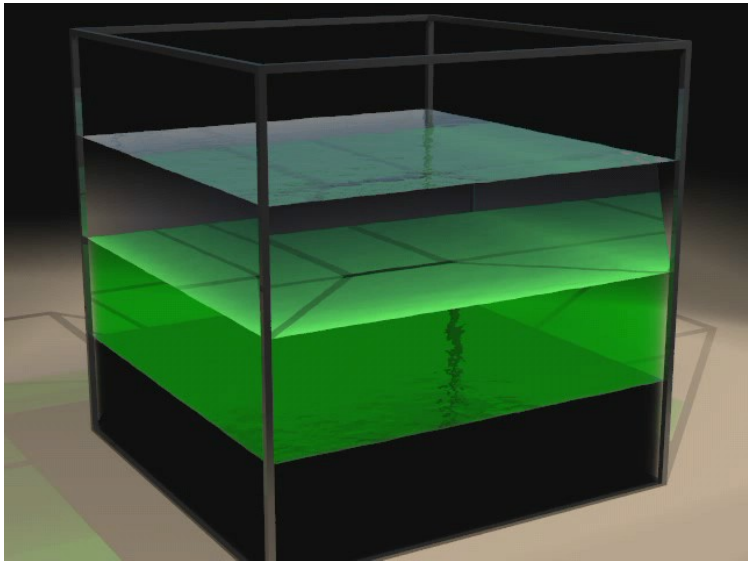
$$S(F)=\operatorname{sgn}(F)$$

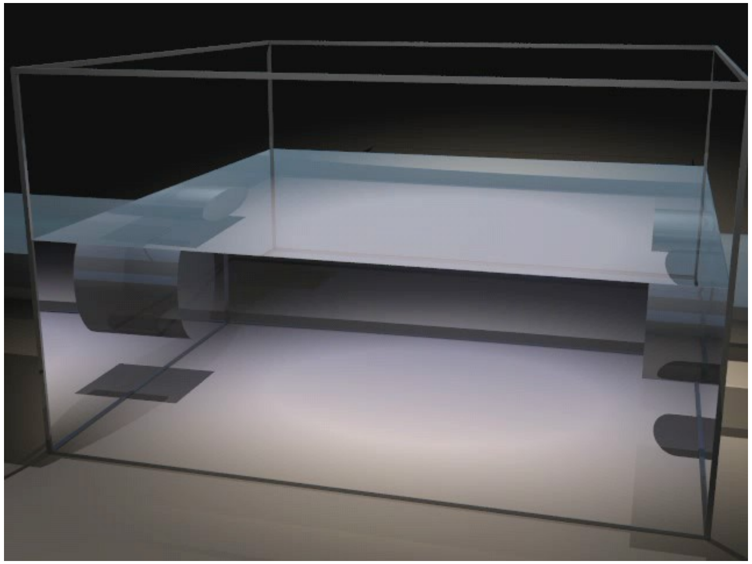
$$S(F)=\frac{F}{\sqrt{F^2+h^2\left|\nabla F\right|^2}}$$

- What kind of function is it? Signed distance from the interface!
- Alas, $\left|\nabla F\right|=1$ is not conserved.
- Relaxing F: τ is pseudo-time (t is not changed)
- Apply alternatively!
- Unfortunately, mass is not conserved in the numeric implementation.
- A better numeric scheme

Level set demo simulations







Numerical implementation of the interfacial source terms in the transport equations

- Example: the normal jump condition due to surface tension can be expressed as an embedded singular source term in the Navier–Stokes equation:

C.f. Level Set

C.f. VOF

$$\rho D_t \mathbf{v} = \rho \mathbf{g} - \nabla p + \nabla \cdot \boldsymbol{\tau} + 2\kappa S \delta(F) \mathbf{n}$$

  - contribution to a single cell in a finite volume model:

$$\iiint_{\text{cell}} 2\kappa S \delta_\varepsilon(F) \nabla F \, dV$$

- Other source terms (latent heat, mass flux) in the transport equations can be treated analogously.

Numerical implementation of the interfacial source terms in the transport equations

$$H_\varepsilon(F) = \begin{cases} 0 & \text{if} \quad F \le -\varepsilon \\ \dfrac{1}{2} + \dfrac{F}{2\varepsilon} + \dfrac{1}{2\pi}\sin\left(\dfrac{\pi \cdot F}{\varepsilon}\right) & \text{if} \quad |F| < \varepsilon \\ 1 & \text{if} \quad F \ge +\varepsilon \end{cases}$$

$$\Downarrow$$

$$\delta_\varepsilon(F) = \begin{cases} 0 & \text{if} \quad F \le -\varepsilon \\ \dfrac{1}{2\varepsilon} + \dfrac{1}{2\varepsilon}\cos\left(\dfrac{\pi \cdot F}{\varepsilon}\right) & \text{if} \quad |F| < \varepsilon \\ 1 & \text{if} \quad F \ge +\varepsilon \end{cases}$$

$$H_\varepsilon(F(t,\mathbf{r})) \xrightarrow[\varepsilon \to 0]{} \chi^{(1)}(t,\mathbf{r})$$

$$\delta_\varepsilon(F) \xrightarrow[\varepsilon \to 0]{} \delta(F)$$

With $\varepsilon = 1.5h$, the interface forces are smeared out to a three-cell thick band

Only first order accurate in h

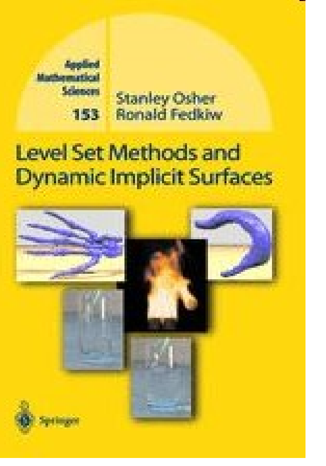
Evaluation criteria for comparison

Not only for VOF and Level Set

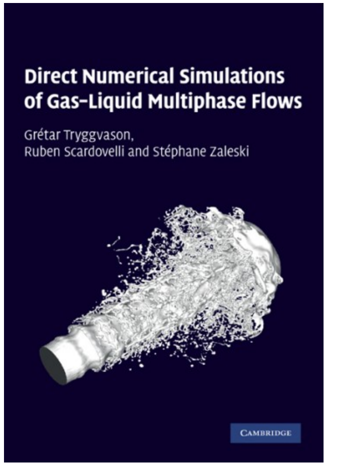
- Ability to
  - conserve mass/volume exactly
  - numerical stability
  - keep interfaces sharp (avoid numerical diffusion and oscillation)
- Ability and complexity to model
  - more than 2 phases
  - phase transitions
  - compressible fluid phases
- Demands on resources
  - number of equations
  - grid spacing
  - grid structure
  - time stepping
  - differentiation schemes
- Limitations of applicability
  - grid types
  - differential schemes
  - accuracy

Recommended books

- Stanley Osher, Ronald Fedkiw:
  Level Set Methods and Dynamic Implicit Surfaces
  Applied Mathematical Sciences, Vol. 153
  (Springer, 2003). ISBN 978-0-387-95482-0
  - Details on the **level set** method



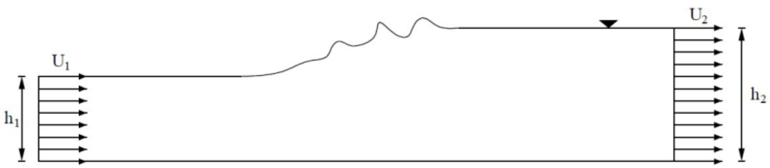
- Grétar Tryggvason, Ruben Scardovelli, Stéphane Zaleski:
  Direct Numerical Simulations of Gas–Liquid Multiphase Flows
  (Cambridge, 2011). ISBN 9780521782401
  - Modern solutions in **VOF** and **front tracking**

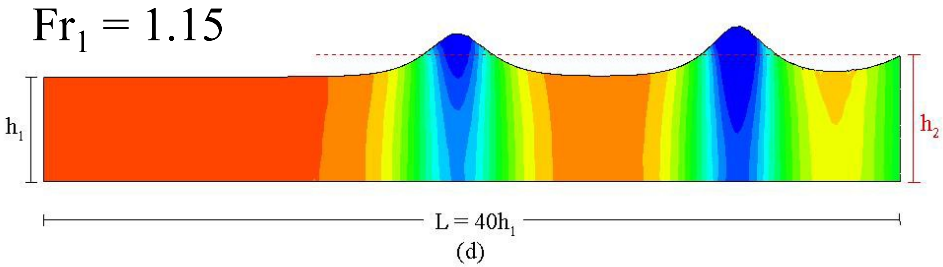


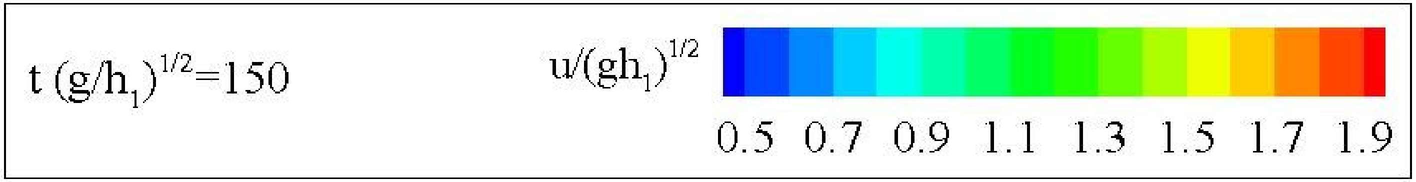
SPH
Smoothed Particle Hydrodynamics

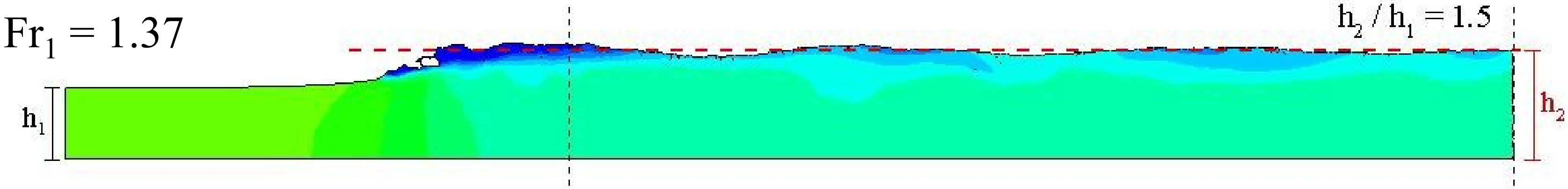
- The other extreme — a *meshless method*:
The fluid is entirely modelled by moving representative fluid particles — fully Lagrangian
- There are no
  - mesh cells
  - interfaces
  - PDE
  - field variables
- Everything is described via ODE's

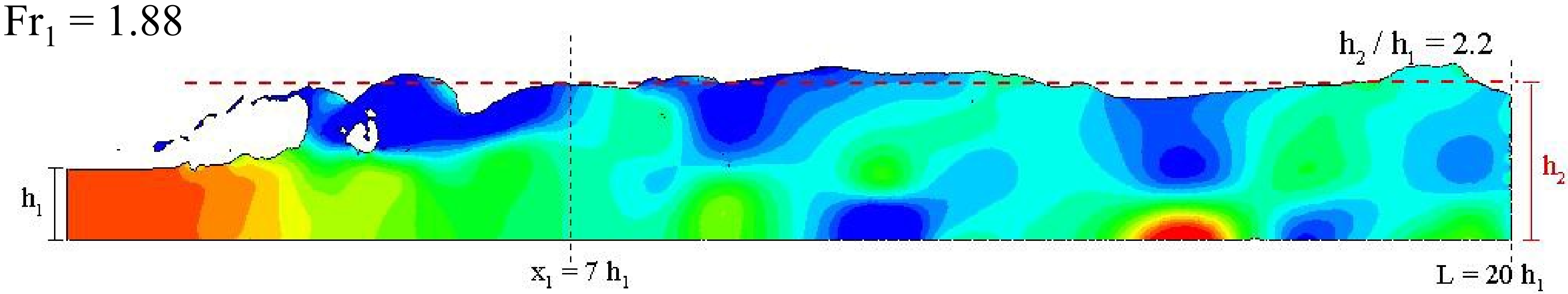
SPH simulation of hydraulic jump



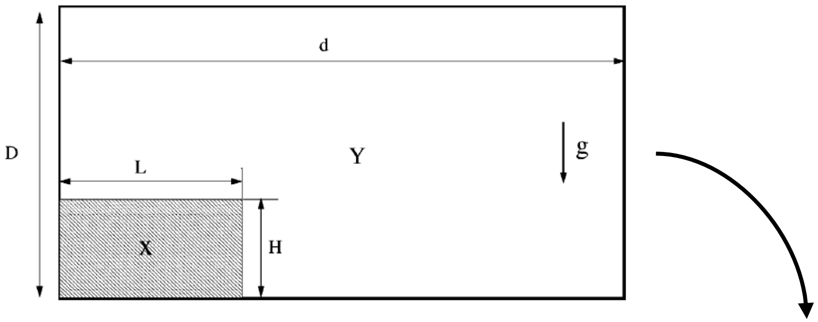


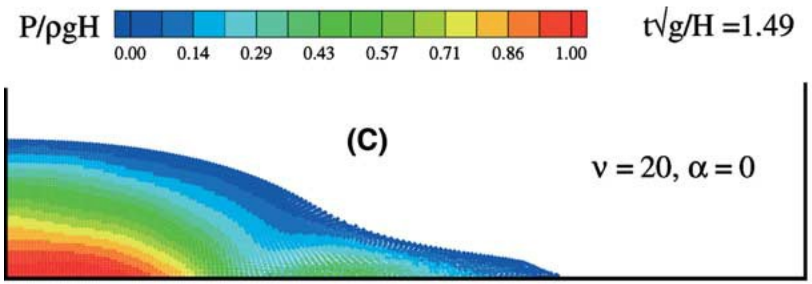


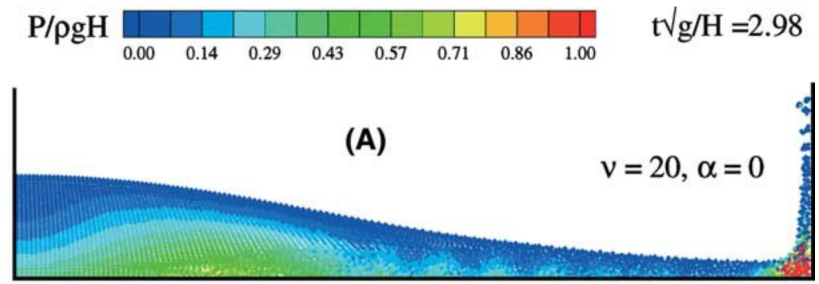


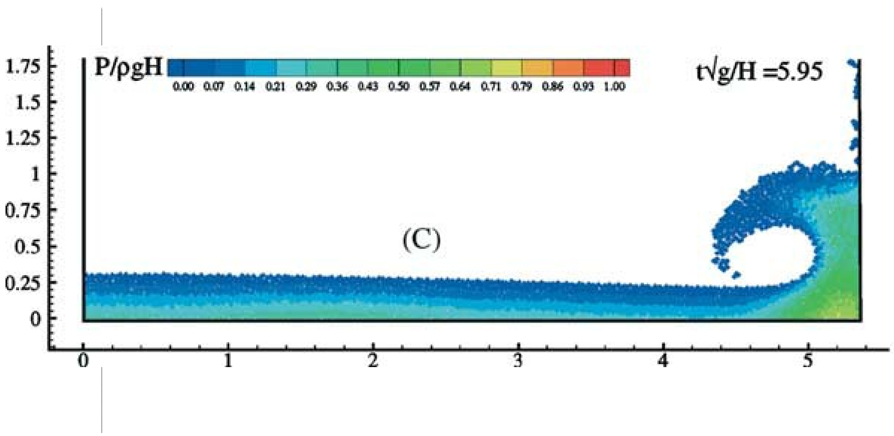


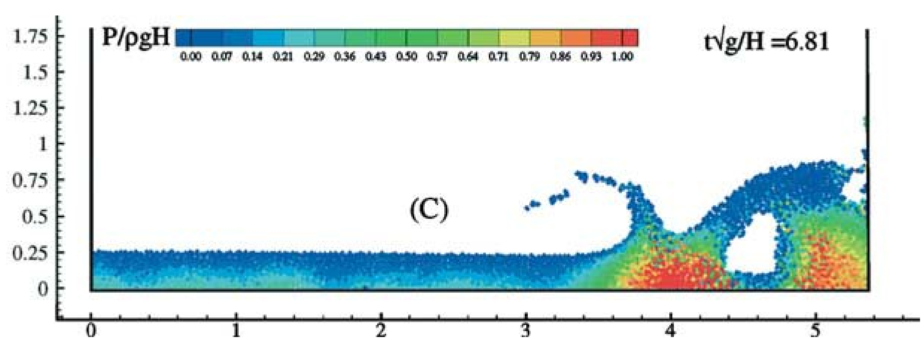
SPH simulation of dam-break



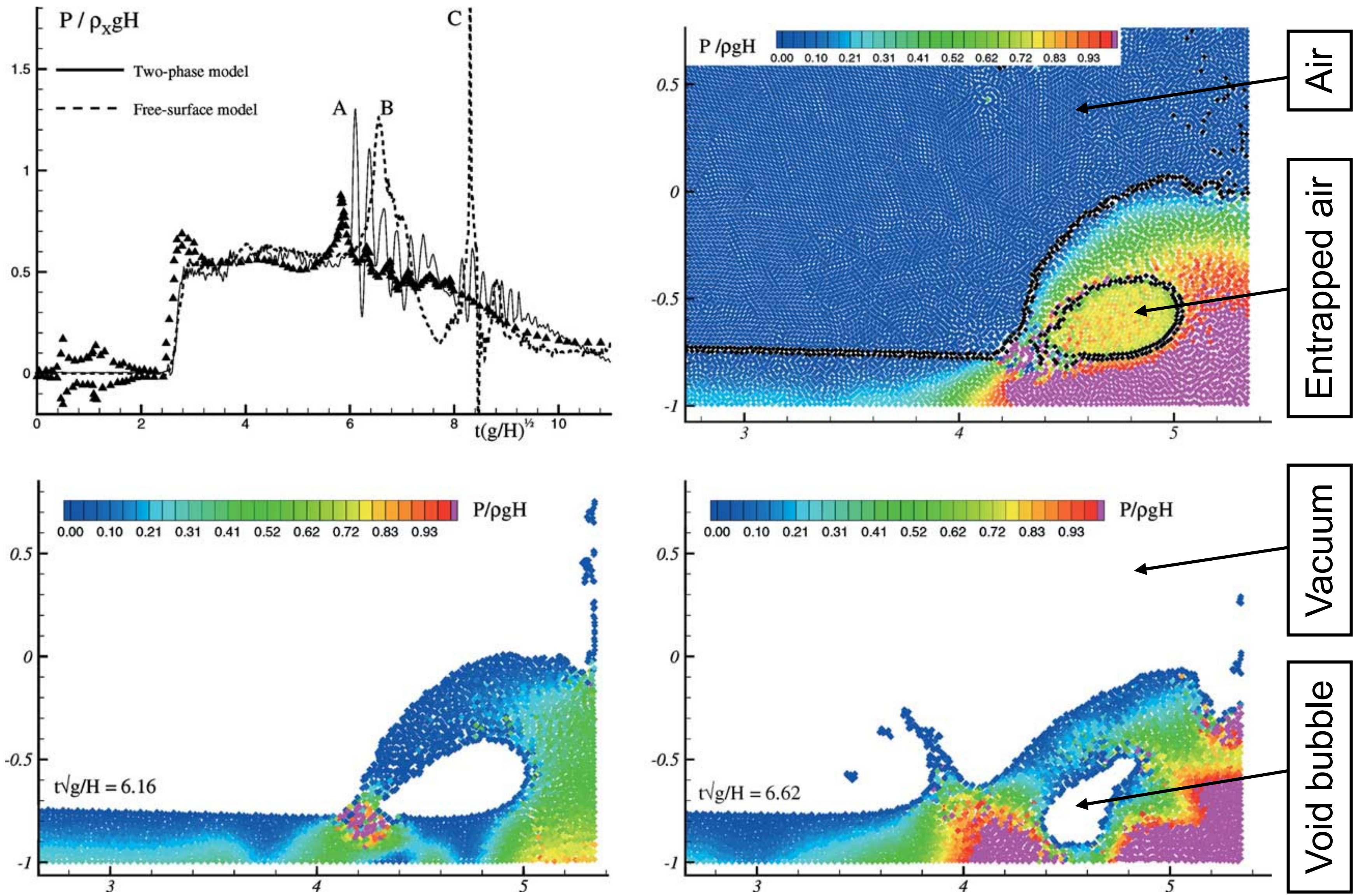








Liquid vs. liquid-gas simulation



SPH demo

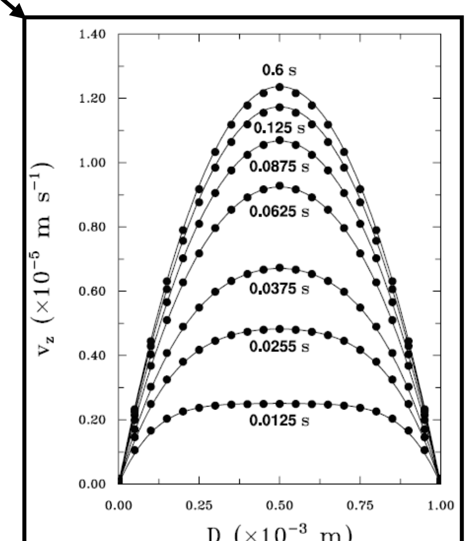
Evaluation of SPH

Advantages

- Conceptually easy
- Best suits problems
  - in which inertia dominates (violent motion, transients, impacts)
    - FSI modelling
  - with free surface or liquid–gas interface
    - Interface develops naturally
- Computationally fast
  - Easy to parallelise
  - Can be adapted to GPU's

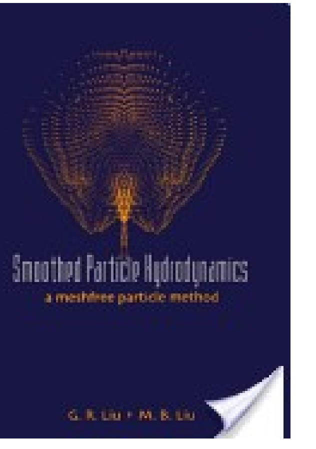
Disadvantages

- High number of particles
- Hard to achieve incompressibility
- Some important boundary conditions are not realised so far

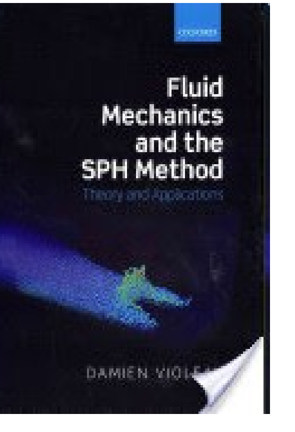


Recommended books on SPH

- G. R. Liu, M. B. Liu:
  Smoothed Particle Hydrodynamics: A Meshfree Particle Method
  (World Scientific, 2003). ISBN 9812564403, ISBN13 9789812564405
  - First book on the **SPH** method



- Damien Violeau:
  Fluid Mechanics and the SPH Method: Theory and Applications
  (OUP Oxford, 2012). ISBN 0199655529, ISBN13 9780199655526
  - Latest achievements in **SPH**



Approaches of `rough´ models

- Multi-fluid (e.g. two-fluid) models
- Mixture models
- Modelling disperse phases

Two key quantities

- <u>Volume fraction</u>

$$\alpha^{(p)}(t,\vec{\mathbf{r}}) \equiv \left\langle \chi^{(p)} \right\rangle =$$

$$= \left(\iiint \sum_p \chi^{(p)}(t,\vec{\mathbf{r}})\, dV \right) \Big/ \left(\iiint dV \right)$$

also known as

– <u>void fraction</u>

in gas–liquid systems

– <u>porosity</u>

in gas–solid systems

- <u>Interfacial area density</u>

$$a(t,\vec{\mathbf{r}}) \equiv$$

$$= \left(\iiint \sum_p \delta\big(F(t,\vec{\mathbf{r}})\big) \cdot \left|\nabla F(t,\vec{\mathbf{r}})\right| dV \right) \Big/ \left(\iiint dV \right)$$

Multi-fluid models

- Fluid elements (computational cells) are large, typically contain both/several phases
- This is described by volume fraction fields, $\alpha^{(p)}$
- Each phase is described by its own phasic transport equations
- A common pressure field is shared
- There is no thermal equilibrium
- The interfaces are not resolved, but inter-phase processes must be parameterised and included in constitutional relations

Balance Equations

$$\sum_p \alpha^{(p)} = 1$$

$$\forall p: \quad \partial_t\left(\alpha^{(p)}\rho^{(p)}\right) + \vec{\nabla}\cdot\left(\alpha^{(p)}\rho^{(p)}\vec{\mathbf{u}}^{(p)}\right) = \sum_{p'}\left(\dot{\rho}^{(p'\to p)} - \dot{\rho}^{(p\to p')}\right)$$

$$\forall p,i: \quad \partial_t\left(\alpha^{(p)}\rho^{(p)}u_i^{(p)}\right) + \vec{\nabla}\cdot\left(\alpha^{(p)}\rho^{(p)}u_i^{(p)}\vec{\mathbf{u}}^{(p)}\right) =$$

$$= \alpha^{(p)}\rho^{(p)}g_i - \alpha^{(p)}\vec{\nabla}p + \vec{\nabla}\cdot\left(\alpha^{(p)}\hat{\boldsymbol{\tau}}^{(p)}\right)$$

$$+ \sum_{p'}\left(\dot{\rho}^{(p'\to p)}u_i^{(p'\to p)} - \dot{\rho}^{(p\to p')}u_i^{(p\to p')} + g_i^{(p\to p')}\right)$$

$$\forall p: \quad \partial_t\left(\alpha^{(p)}\rho^{(p)}h^{(p)}\right) + \vec{\nabla}\cdot\left(\alpha^{(p)}\rho^{(p)}h^{(p)}\vec{\mathbf{u}}^{(p)}\right) =$$

$$= \alpha^{(p)}\partial_t p - \vec{\nabla}\cdot\vec{\mathbf{j}}_h^{(p)} + \dot{q}_h^{(p)} + \left(\alpha^{(p)}\hat{\boldsymbol{\tau}}^{(p)}\right)\bullet\left(\vec{\nabla}\vec{\mathbf{u}}^{(p)}\right)$$

$$+ \sum_{p'}\left(\dot{\rho}^{(p'\to p)}h^{(p'\to p)} - \dot{\rho}^{(p\to p')}h^{(p\to p')} + \dot{q}_h^{(p\to p')}\right)$$

Inter-phase processes

Constitutive Relations

- Primary field varaibles:

$$\alpha^{(p)}(t,\vec{\mathbf{r}}),\ \vec{\mathbf{u}}^{(p)}(t,\vec{\mathbf{r}}),\ p(t,\vec{\mathbf{r}}),\ h^{(p)}(t,\vec{\mathbf{r}})$$

- Constitutive equations
  - Intrinsic:

$$\rho^{(p)}(p,h^{(p)})$$

$$\mu^{(p)}(p,h^{(p)})$$

$$k^{(p)}(p,h^{(p)})$$

  - Heat sources: $\dot{q}_h^{(p)}$
  - Phase transition fluxes
    - Inter-phase processes:

$$\dot{\rho}^{(p'\to p)}, \vec{\mathbf{u}}^{(p'\to p)}, h^{(p\to p')},$$

    - Work $g_i^{(p\to p')},$
    - Heat transfer $\dot{q}_h^{(p\to p')}$

It is possible to generalise to multi-component phases

Pros and Cons

TOO MANY EQUATIONS

- Intrinsic constitutive equations are the same as the single-phase ones
- One needs a lot of external constitutive equations
- Some of these require empirical correlations
- Sometimes there is not enough experimental data to establish such correlations
- Risk of unsubstantiated assumptions
- High computational demand (w.r.t. the one-fluid models)
- Low computational demand (w.r.t. fine models)
- Flexibility

If it makes sense, some simplification can be achieved by assuming thermal equilibrium among the phases

Mixture model

- Derived by averaging and using simplifying assumptions
- The mixture is considered as a single fluid
- Common T and p
- The interfaces are ignored
- All interface processes are transferred to constitutive laws

$$\rho(t,\vec{\mathbf{r}}) \equiv \langle \rho \rangle = \left(\iiint \sum_p \chi^{(p)}(t,\vec{\mathbf{r}})\rho^{(p)}(t,\vec{\mathbf{r}})\, dV \right) \Big/ \left(\iiint dV \right)$$

$$\vec{\mathbf{u}}(t,\vec{\mathbf{r}}) \equiv \langle \rho \vec{\mathbf{u}} \rangle \big/ \rho(t,\vec{\mathbf{r}}) = \left(\iiint \sum_p \chi^{(p)}(t,\vec{\mathbf{r}})\rho^{(p)}(t,\vec{\mathbf{r}})\vec{\mathbf{u}}(t,\vec{\mathbf{r}})\, dV \right) \Big/ \rho(t,\vec{\mathbf{r}})$$

$$e(t,\vec{\mathbf{r}}) \equiv \langle \rho e \rangle \big/ \rho(t,\vec{\mathbf{r}}) = \left(\iiint \sum_p \chi^{(p)}(t,\vec{\mathbf{r}})\rho^{(p)}(t,\vec{\mathbf{r}})\, e(t,\vec{\mathbf{r}})\, dV \right) \Big/ \rho(t,\vec{\mathbf{r}})$$

Pros and Cons

TOO FEW EQUATIONS

- Do not describe small-scale phenomena at all
- The external constitutive equations must be based on empirical correlations
- Not even the intrinsic constitutive equations are general, they are problem-dependent
- Too much constrained to describe adequately the flow phenomena
- Lowest computational demand (w.r.t. fine models)

Remedies

It is possible to extend the model by adding new primary fields to the model in addition to $p(t,\vec{\mathbf{r}})$, $\vec{\mathbf{u}}(t,\vec{\mathbf{r}})$ and $T(t,\vec{\mathbf{r}})$

Example: volume fraction field, $\alpha^{(p)}$

$$\alpha^{(p)}(t,\vec{\mathbf{r}}) \equiv \left\langle \chi^{(p)} \right\rangle =$$

$$= \left(\iiint \sum_p \chi^{(p)}(t,\vec{\mathbf{r}})\, dV \right) \Big/ \left(\iiint dV \right)$$

1. Homogenous model
2. Generalised homogenous model
3. Slip model
4. Non-equilibrium model
5. Diffusion model

- These include more constitutive equations and thus need more correlations
- The consistency of the system cannot be assured

Modelling Disperse Phases

The previous models were based on the ‘Eulerian’ approach (time- and position-dependent fields)

- Ambient fluid: single-phase ‘Eulerian’ model
- Disperse phase — ‘Lagrangian’ model:
  - Establish equation of motion of particles subject to fluid forces
  - Solve this for each particle, and follow their path in the fluid
  - Draw conclusions from statistics upon particles

Mixed ‘Eulerian–Lagrangian’ approach

Degrees of Disperse Phase Modelling

Increasing particle loading

1. Flow→particle: Track individual particles subject to ambient flow
2. Particle↔particle coupling: include interactions
3. Flow↔particles coupling: include effect of particles on the ambient flow
4. Consider particle–particle contacts

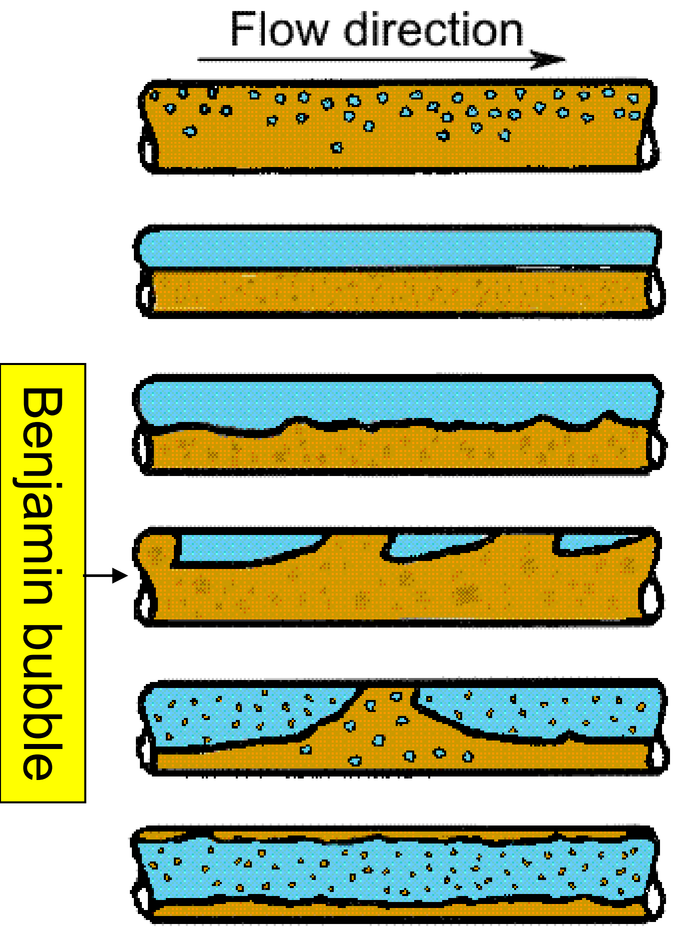
Features of Disperse Phase Modelling

- Effects of various fluid dynamical actions
- Particle-wall interactions, depositions
- Sedimentation
- Bubbles and drops:
  - Growth and collapse
  - Coalescence and breakup
- Studying varying particle size distribution

Multiphase pipe flows

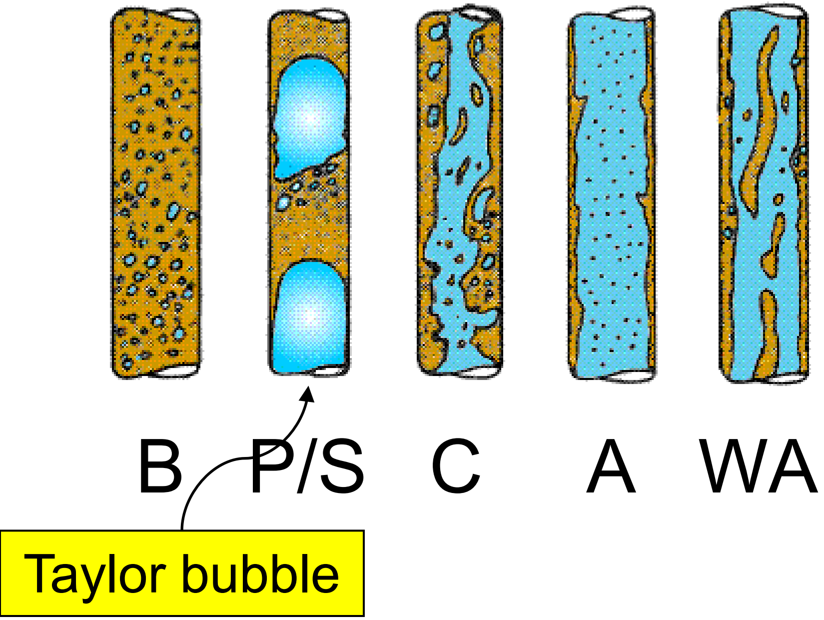
- Physical phenomena
- Modelling approaches

Horizontal gas-liquid flow patterns



- Dispersed Bubble Flow
- Stratified Flow
- Stratified–Wavy Flow
- Plug Flow
- Slug Flow
- Annular–Dispersed Flow

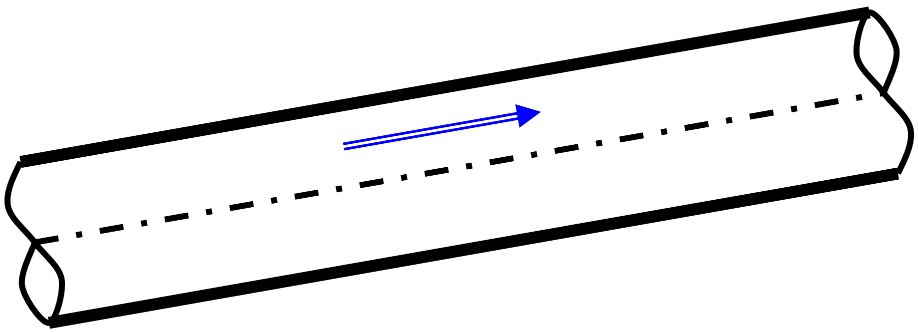
Vertical gas-liquid flow patterns



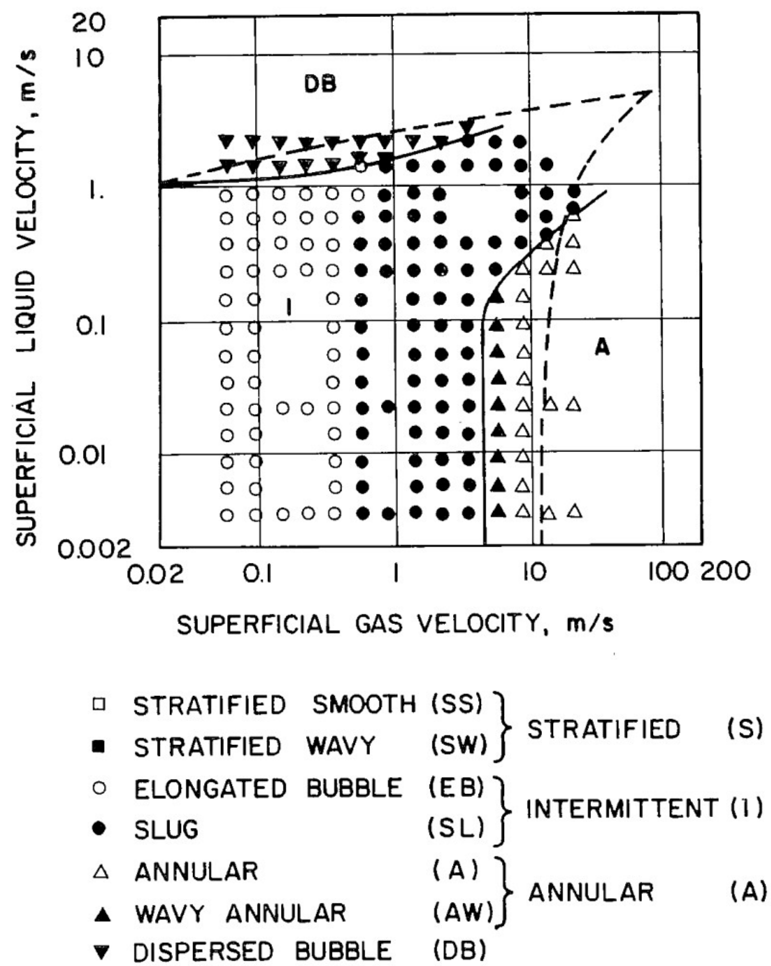
- Bubble Flow
- Plug or Slug Flow
- Churn Flow
- Annular Flow
- Wispy Annular Flow

http://www.thermopedia.com/

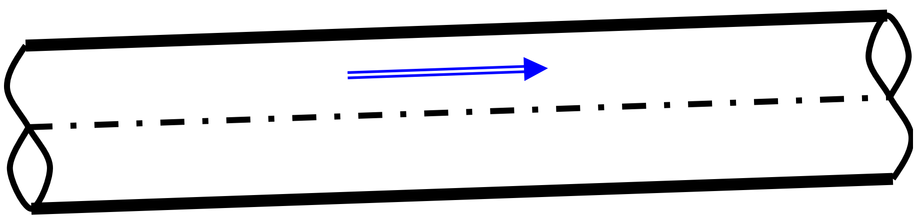
The effect of pipe inclination



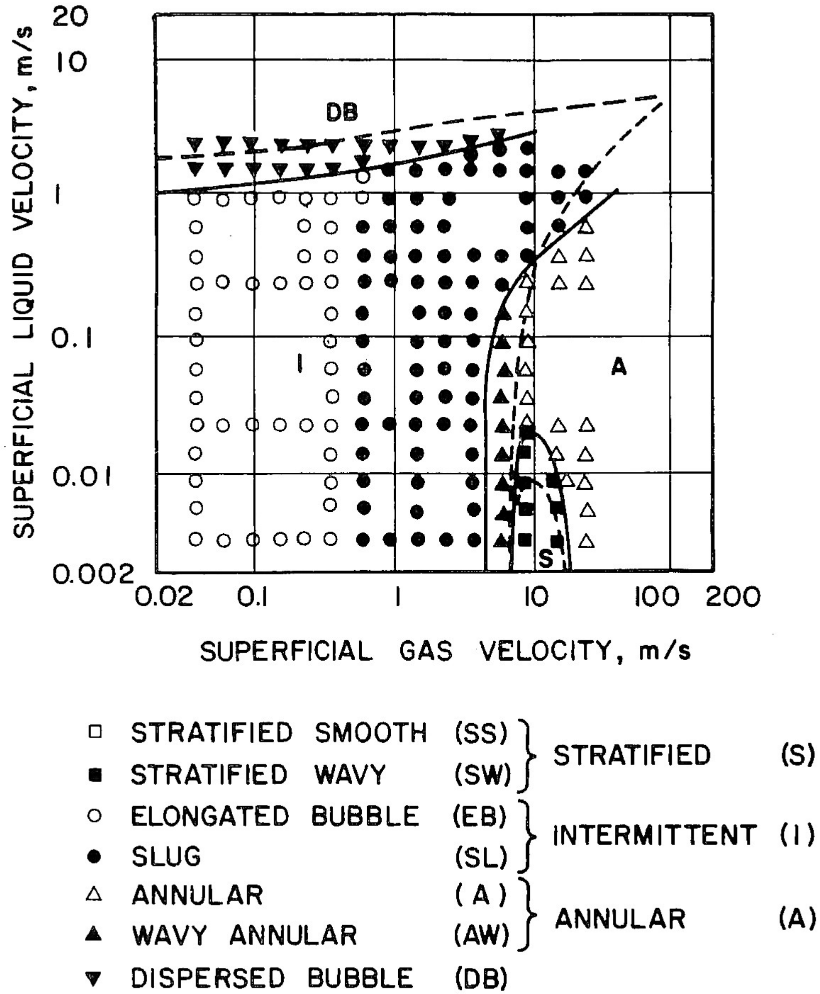
$\Theta = +10°$



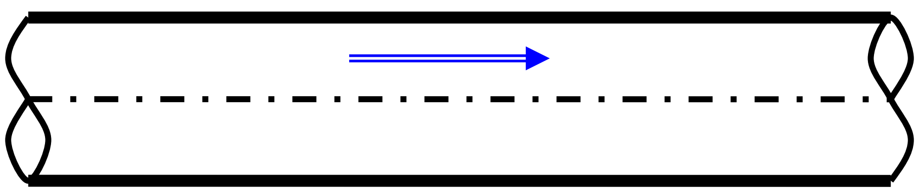
The effect of pipe inclination



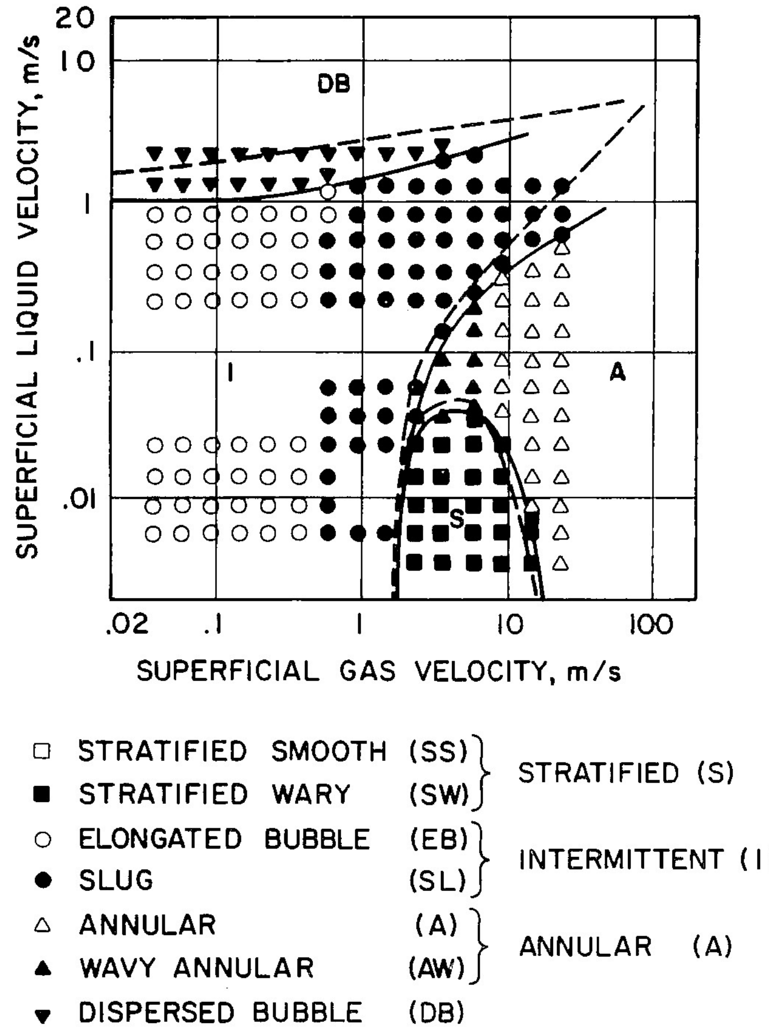
$\Theta = +2°$



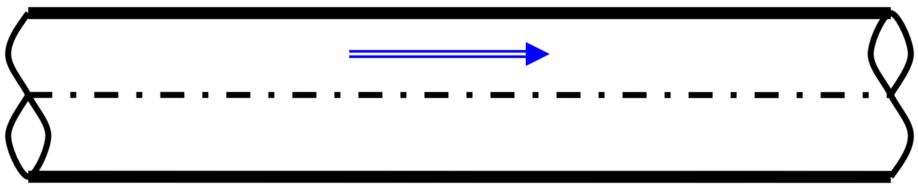
The effect of pipe inclination



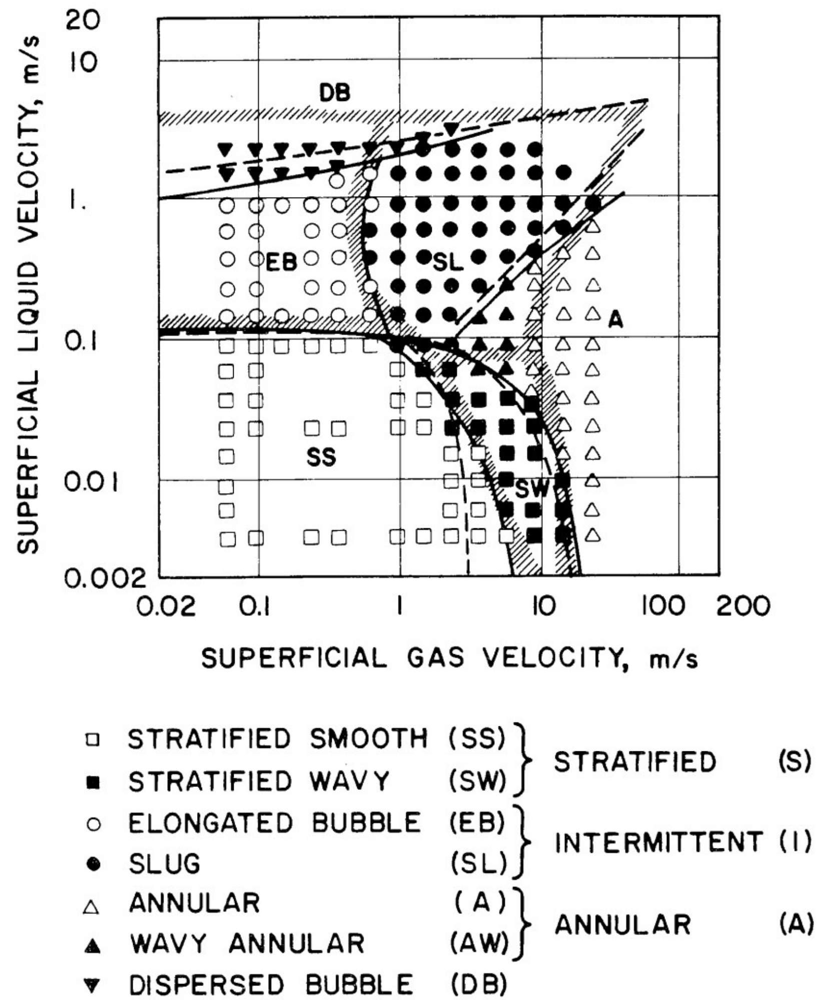
$\Theta = +0.25°$



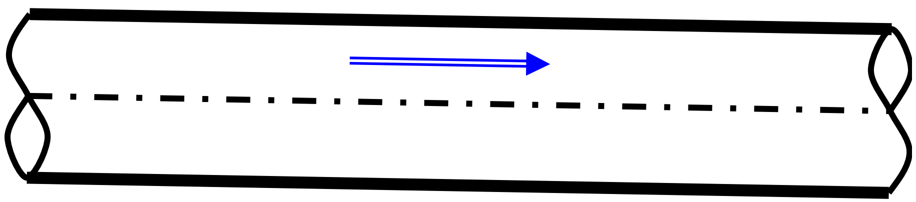
The effect of pipe inclination



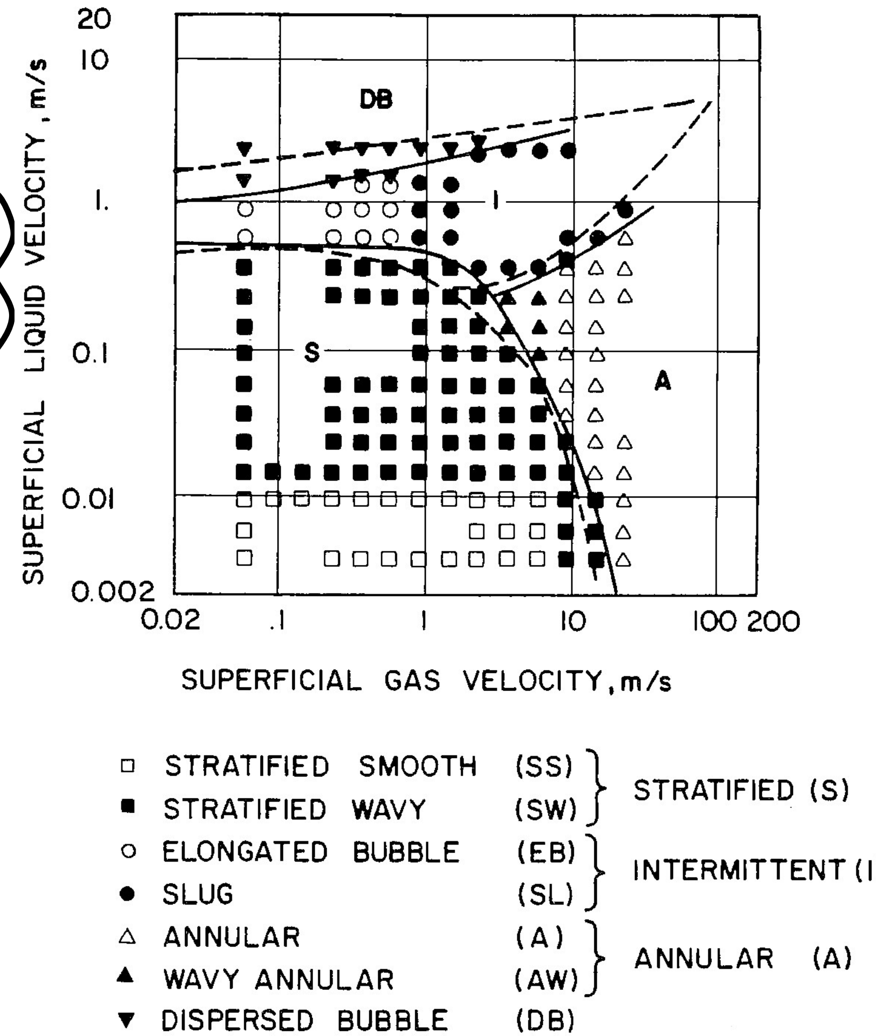
Θ = 0°



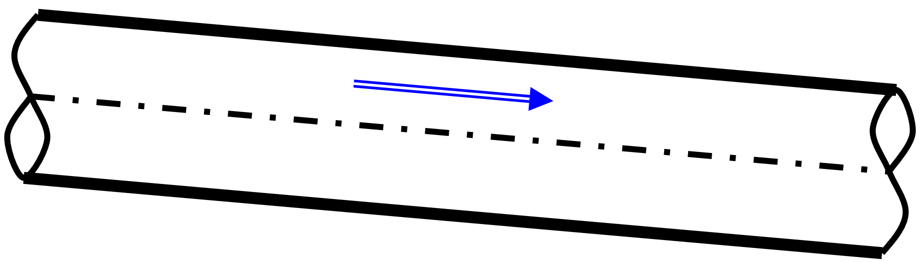
The effect of pipe inclination



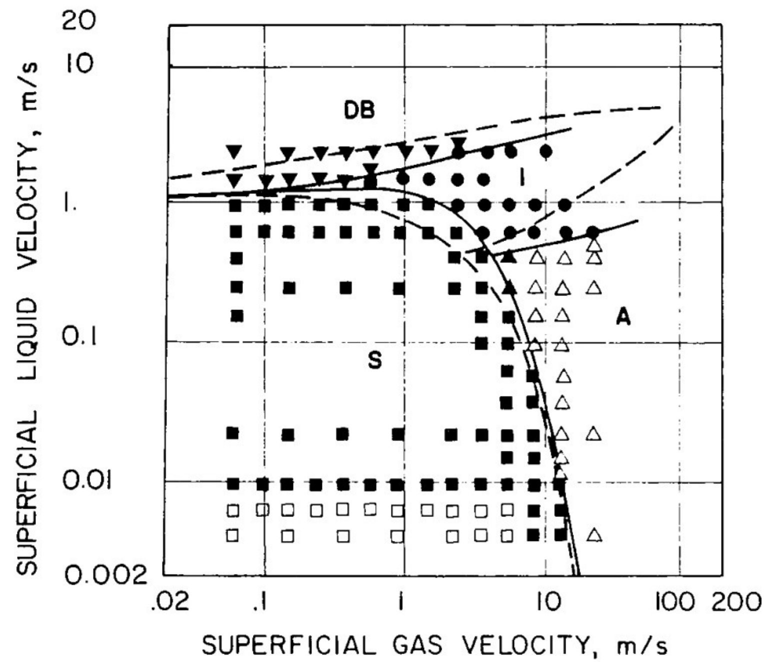
$\Theta = -1°$



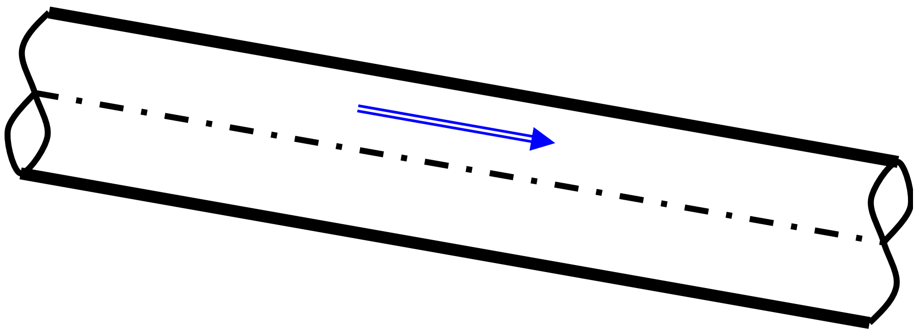
The effect of pipe inclination



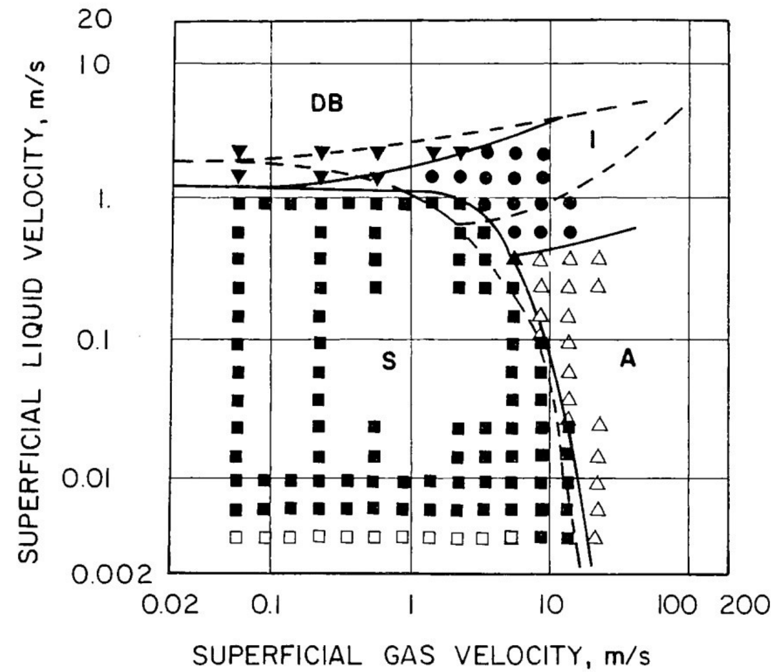
$\Theta = -5°$



The effect of pipe inclination



$\Theta = -10°$



□	STRATIFIED SMOOTH	(SS)	STRATIFIED	(S)
■	STRATIFIED WAVY	(SW)		
○	ELONGATED BUBBLE	(EB)	INTERMITTENT	(I)
●	SLUG	(SL)		
△	ANNULAR	(A)	ANNULAR	(A)
▲	WAVY ANNULAR	(AW)		
▼	DISPERSED BUBBLE	(DB)		

- Relative flow directions
  - Co-current flow (as shown above)
  - Counter-current flows (one of the mass flow rates is negative): some of the flow patterns exist with opposite flow directions too
- Somewhat analogous flow patterns can be identified in liquid-liquid, liquid-solid and gas-solid systems

- Even more complex flow patterns in three phase pipe flows
- Flow classification is
  - somewhat arbitrary and subjective in pipes
  - hardly possible in 3D containers
- Further points to observe:
  - Heat transfer phenomena
  - Phase transition phenomena

Pipe flow modelling alternatives

- Flow patterns
- Flow regimes
- Flow pattern maps
- Tasks:
  - Model flow region boundaries
  - Model flow behaviour within each flow region

Create a single one fluid model that can correctly reflect fluid behaviour in all flow regimes and thus automatically describes flow pattern transitions

Parameters of one-phase pipe flow

Control (input) parameters:

- Pipe geometry
  - shape
  - size
  - inclination
  - wall roughness
- Mass flow rate
- Fluid properties
- External heat source

Measured (output) parameters:

- Pressure drop
- Transported heat

Parameters of two-phase pipe flow

Control (input) parameters:

- Pipe geometry
  - shape
  - size
  - inclination
  - wall roughness
- Mass flow rates
- Fluid properties
- External heat source

Measured (output) parameters:

- Pressure drop
- Volume (void) fraction
- Interfacial area density
- Transported heat

Model variables in pipe systems

- Cross sectional integral quantities
  - linear densities
  - flow rates
- Cross sectional average (‘mean`) quantities
  - ‘mean` densities
  - ‘mean` fluxes

Purpose: reduction of independent variables: $(t,x,y,z) \to (t,x)$

Definitions and measurements of void fraction

- Local (time averaged)
- Chordal
- Cross sectional averaged
- Volume averaged