Multi-Phase Flow Modelling

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Outline

Objective

- Present physical modelling baseline and implementation details of multi-phase and free surface flow algorithms

Topics

- Overview of multi-phase modelling: Levels of approximation
- Eulerian multi-phase flow model
- Population balance modelling
- Volume-of-Fluid (VOF) flow model
- Thin liquid film model
- Lagrangian particle tracking: Discrete particle model
- Free surface tracking model

Multi-Phase Flow Modelling

Physical Modelling of Multi-Phase Flows

- Presence of multiple phases in the domain of interest. Inter-phase coupling is of primary interest: momentum transfer between phases
- Phases described as a **continuous phase** (or background phase) and a **dispersed phases**, interacting with the continuous phase
- Levels of approximation: **Coupled Approach**
  - Medium volume fraction: **Euler-Euler approach**. Phases are considered as inter-penetrating continua occupying the same volume. Equations are solved in a fully coupled manner in Eulerian formulation
  - Low volume fraction: **Euler-Lagrange approach**. Continuous phase is treated in the Eulerian manner, while the dispersed phase is represented by a population of discrete parcels tracked in a Lagrangian manner
  - **Free surface flow model** is a special case of the Euler-Euler model, with a single momentum equation and no phase inter-penetration. This is the only reliable approach for high volume fraction
- Levels of approximation: **Decoupled Approach**
  - Lagrangian particle tracking with uni-directional momentum transfer
  - Wall film model: liquid transport along a curved surface in 3-D

Eulerian Multi-Phase Model

Eulerian Multi-Phase Model

- The system is considered as two (or more) inter-penetrating continua filling the computational domain
- Phase concentration followed by solving the **volume fraction equation** for α_ϕ, which is derived from dispersed phase continuity
- Each phase is represented by its momentum equation. Phases exchange momentum in a two-way manner: inter-phase lift and drag terms
- Pressure is considered to be shared between phases
- Equation set derived using **conditional averaging** technique, (Dopazo, 1977)

Eulerian Multi-Phase Model

Equation set for Eulerian Multi-Phase Flow

- Phase continuity equation

$$\frac{\partial \alpha_\phi}{\partial t} + \nabla \bullet (\overline{\mathbf{u}}_\phi \alpha_\phi) = 0$$

- Phase momentum equation

$$\frac{\partial (\alpha_\phi \overline{\mathbf{u}}_\phi)}{\partial t} + \nabla \bullet (\alpha_\phi \overline{\mathbf{u}}_\phi \overline{\mathbf{u}}_\phi) + \nabla \bullet (\alpha_\phi \overline{\mathbf{R}}_\phi^{eff}) = -\frac{\alpha_\phi}{\rho_\phi} \nabla \overline{p} + \alpha_\phi \mathbf{g} + \frac{\mathbf{M}_\phi}{\rho_\phi}$$

- Defining volume velocity as a sum of phase velocities

$$\mathbf{u} = \sum_\phi \alpha_\phi \overline{\mathbf{u}}_\phi$$

- Volume continuity equation

$$\nabla \bullet \mathbf{u} = 0$$

Eulerian Multi-Phase Model

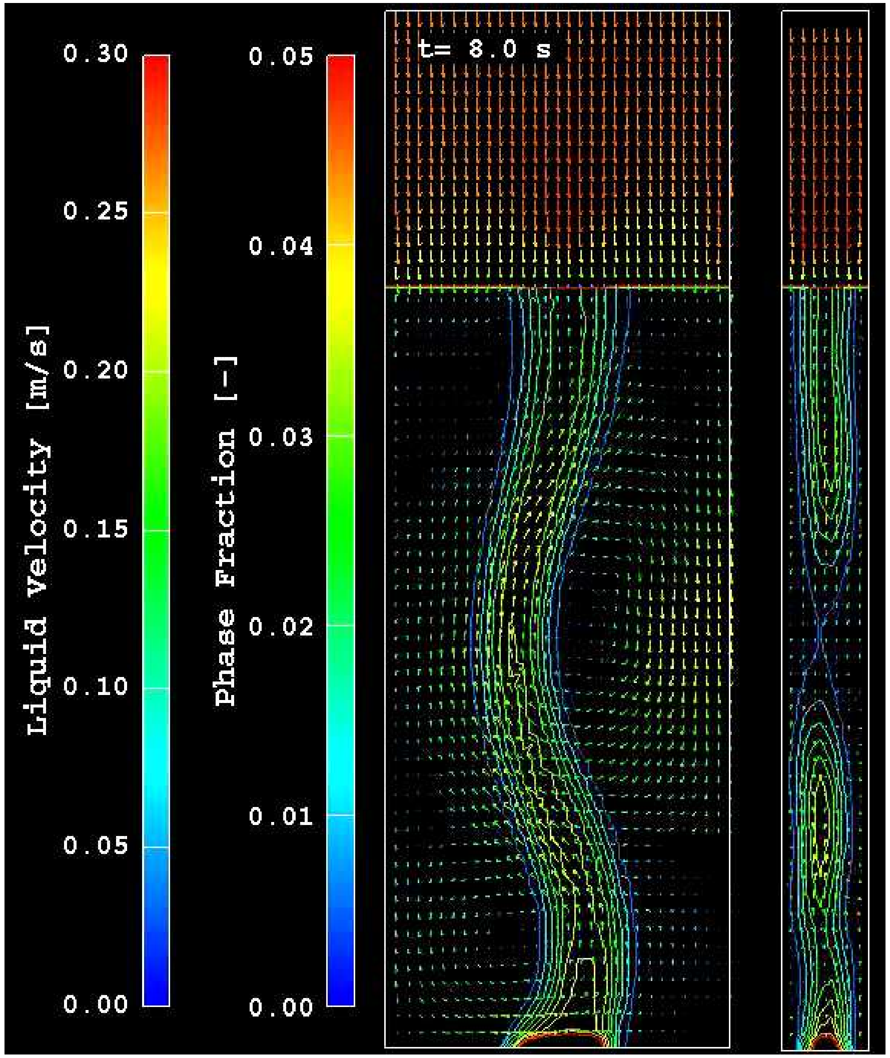
Eulerian Multi-Phase Model

- Main problem in derivation is calculating multiple $\overline{\mathbf{u}}_\phi$ from a single pressure equation: one pressure provides a single set of fluxes
- Solution: reformulated phase fraction equation (Rusche, 2003). Dropping subscript and reducing to a two-phase system for simplicity

$$\frac{\partial \alpha}{\partial t} + \nabla\bullet(\mathbf{u}\alpha) + \nabla\bullet[(\mathbf{u}_\alpha - \mathbf{u}_\beta)\,\alpha\,(1-\alpha)] = 0$$

  The final term contains relative phase velocity and appears on the interface
- Reformulated momentum equation also uses volumetric velocity in the convection term, avoiding issues with interpolation of phase fraction
- Partial elimination of drag terms for stability of momentum coupling

Eulerian Multi-Phase Model



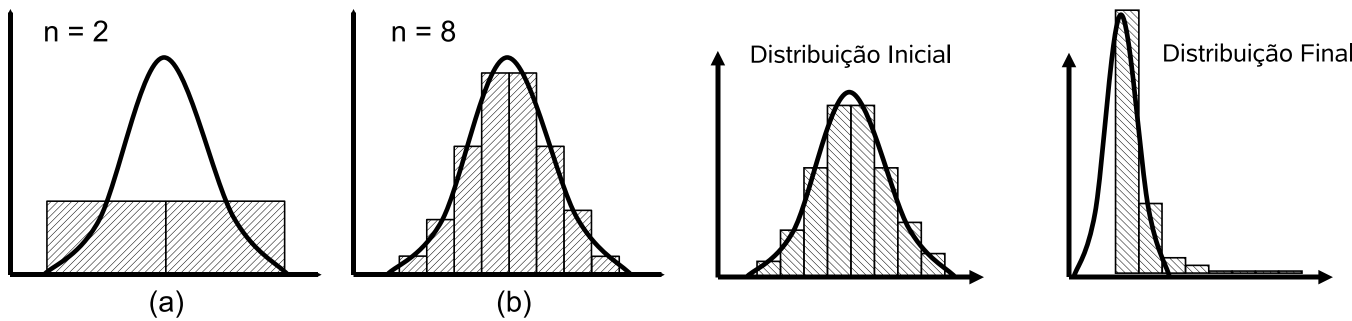
Example: Bubble Plume

- Bubble column experiment: Gomes et al. 1998
- Air bubbles are injected at bottom plate. Maximum flow velocity is larger than injection velocity because of recirculation
- Cases contains free surface: need to handle $\alpha = 0$ condition in the equation set
- Simulations: Henrik Rusche, PhD

Multiphase Flows

Multiphase Flow: Population Balance Model

- Inter-phase momentum transfer (drag, lift, virtual mass) depends on characteristic radius of the dispersed phase $\rightarrow$ which is not constant!
- Accounting for **droplet breakup and aggregation** implies knowledge of droplet size distribution: heterogenous multiphase flow
- Hybrid classes-moments method: describe distribution in a set of size buckets

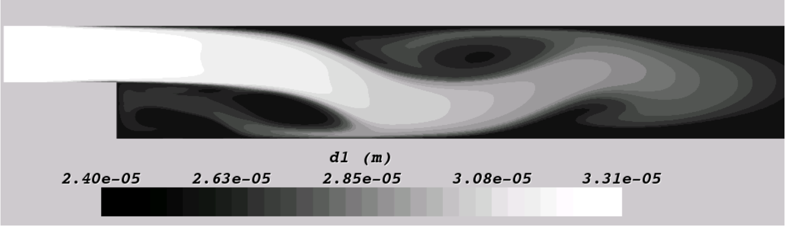


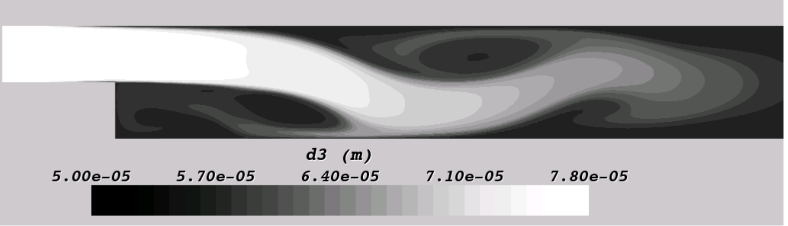
  - **Fixed pivot approximation**: 150-250 pivots needed to avoid loss of precision
  - **Quadrature approximation**: optimal adaptive weights and abscissas. Five to six quadrature points sufficient for good accuracy: DQMOM model
- Depending on model, momentum equation may be shared between abscissas
- System acts as n-phase multi-phase system with coupling and “phase” exchange

Multiphase Flows

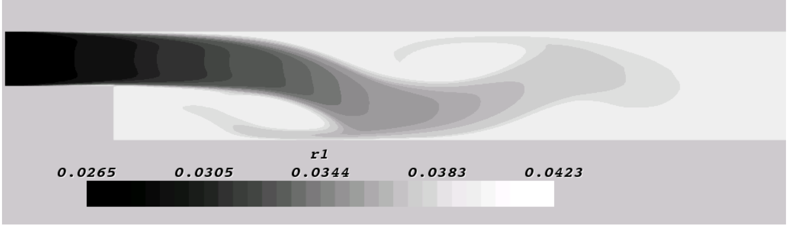
Example: Backward-Facing Step Flow, Dominant Breakage

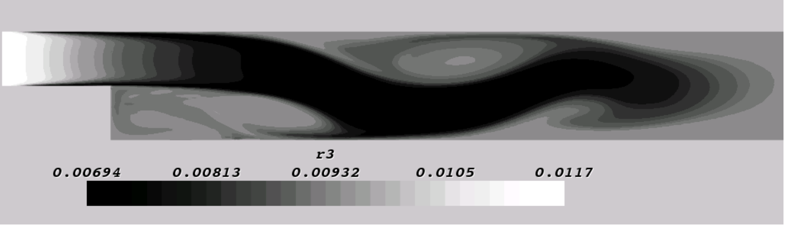
- In dominant breakage, dispersed phase distribution is moving to the left
  - Dropping value of abscissas
  - Increasing volume fraction of “small droplet” phase
- Characteristic diameter for first and third abscissa





- Volume fraction for first and third abscissa (= product of abscissa and weight)

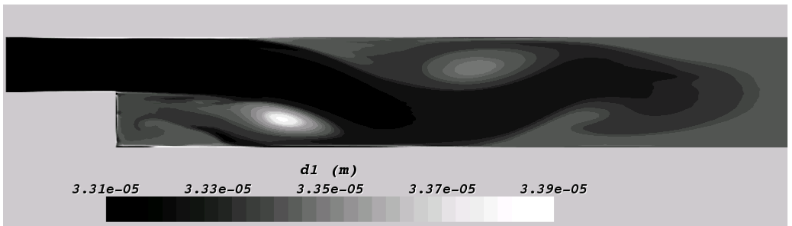


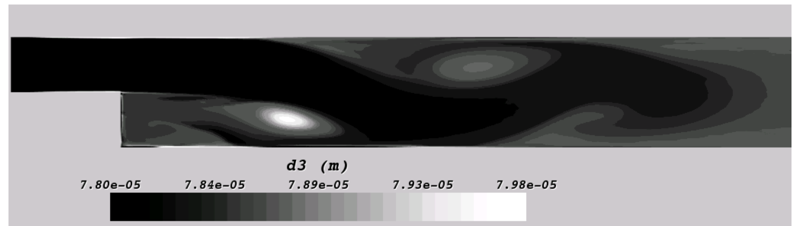


Multiphase Flows

Example: Backward-Facing Step Flow, Dominant Aggregation

- In dominant breakage, dispersed phase distribution is moving to the right
  - Increasing value of abscissas
  - Increasing volume fraction of “large droplet” phase
- Characteristic diameter for first and third abscissa





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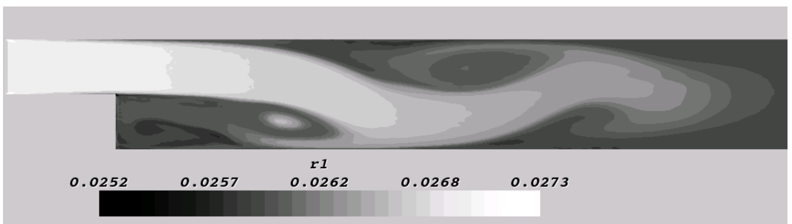
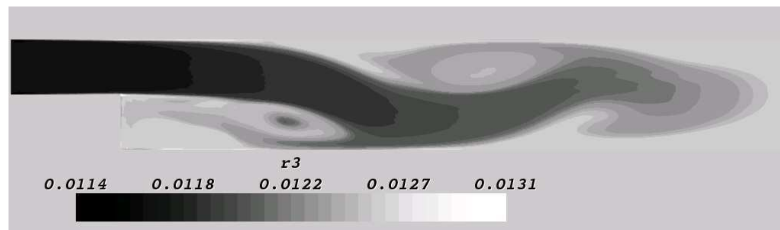




Free Surface Flow Model

Volume-of-Fluid Model

- **Volume of Fluid Model**: variant of multi-phase model preserving phase interface
- Immiscible condition combines momentum equations: no inter-penetrating continua, no inter-phase drag terms
- Formulation follows Eulerian multi-phase model, but combines momentum equations since phases do not inter-penetrate
- Phase continuity equation with volume fraction variable γ

$$\frac{\partial \gamma}{\partial t} + \nabla_\bullet(\mathbf{u}\gamma) = 0$$

- Combined momentum equation

$$\frac{\partial(\rho\mathbf{u})}{\partial t} + \nabla_\bullet(\rho\mathbf{u}\mathbf{u}) - \nabla_\bullet\boldsymbol{\sigma} = -\nabla p + \rho\mathbf{f} + \sigma\kappa\nabla\gamma$$

Note the presence of **surface tension term**, depending on curvature of free surface. Curvature is calculated from γ field

Free Surface Flow Model

Free Surface Flow Model

- Phases are considered a single continuum, with jump in properties at the interface

$$\mathbf{u} = \gamma \mathbf{u}_1 + (1 - \gamma)\mathbf{u}_2$$

$$\rho = \gamma \rho_1 + (1 - \gamma)\rho_2$$

$$\nu = \gamma \nu_1 + (1 - \gamma)\nu_2$$

Numerical Considerations: Sharp Interface

- Preserving sharpness of free surface is paramount
  - **Compressive numerics** on $\nabla\bullet(\mathbf{u}\gamma)$ term: Onno Ubbink PhD, 1997. Problems with parasitic velocities and dominant surface tension
  - **Relative velocity formulation**, Rusche PhD 2003: use the Eulerian two-phase form of the phase fraction equation, but manufacture relative velocity term

$$\frac{\partial \alpha}{\partial t} + \nabla\bullet(\mathbf{u}\alpha) + \nabla\bullet[\mathbf{u}_r\, \alpha\, (1 - \alpha)] = 0$$

    where $\mathbf{u}_r$ is a function of interface normal $\nabla\gamma$

Free Surface Flow Model

Numerical Considerations: Pressure Handling

- Pressure field contains several tricky terms
  - Gravity contribution: hydrostatic pressure from $\rho\mathbf{f}$
  - Surface tension term: in distributed form $\sigma\kappa\nabla\gamma$
- To ensure smooth numerics, both terms are removed from momentum equation and built into the pressure. This replaces static pressure with its dynamic (piezometric) equivalent; static pressure can be recovered separately

Numerical Considerations: Surface Curvature and Surface Tension

- Surface curvature calculated from volume fraction gradient

$$\kappa = \nabla\bullet\left(\frac{\nabla\gamma}{|\nabla\gamma|}\right)$$

- Distributed form of surface tension pressure jump

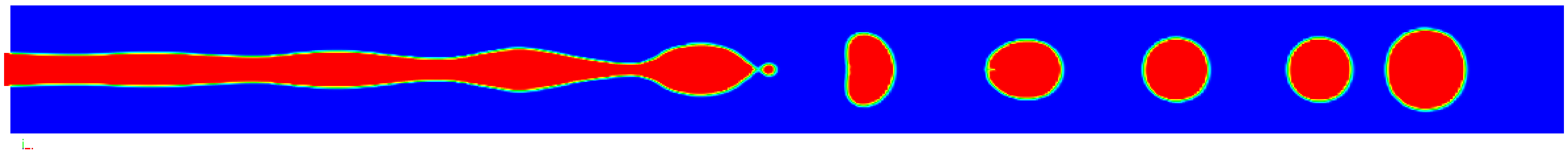
$$\int_{S(t)} \sigma\kappa'\mathbf{n}'\delta(\mathbf{x}-\mathbf{x}')\,dS \approx \sigma\kappa\nabla\gamma$$

Free Surface Flow Model

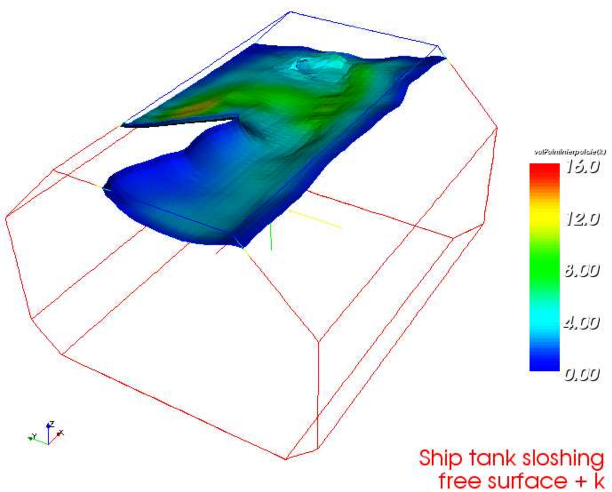
Examples

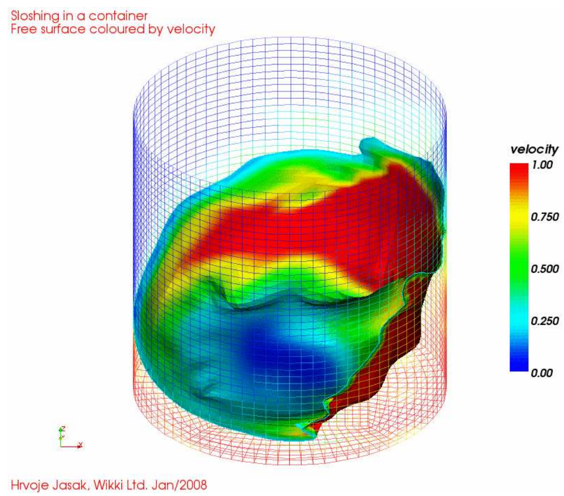
- Efficient handling of interface breakup
- Accurate handling of dominant surface tension: no parasitic velocity

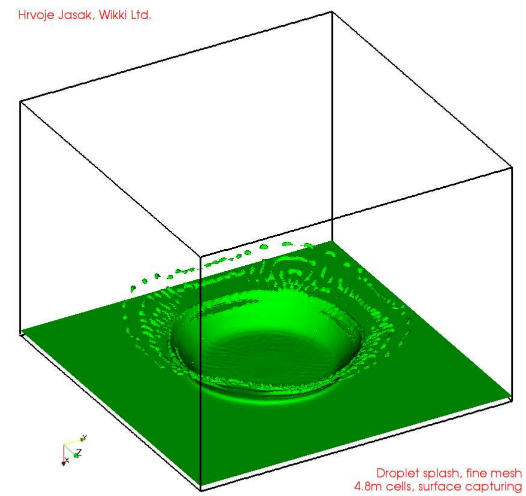
Ink-Jet Printer Nozzle, $d = 20\mu\mathrm{m}$: Breakup Under Dominant Surface Tension



Complex Surface Breakup Phenomena: Sloshing and wet wall impact



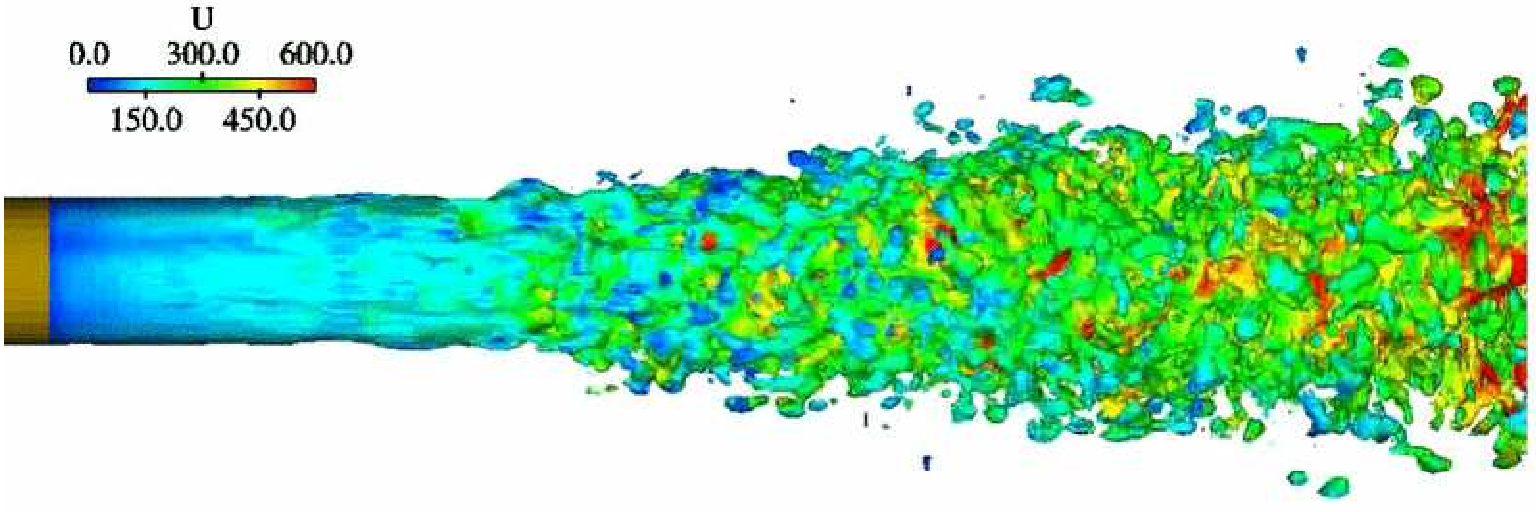




Free Surface Flow Model

Examples: LES of a Diesel Injector

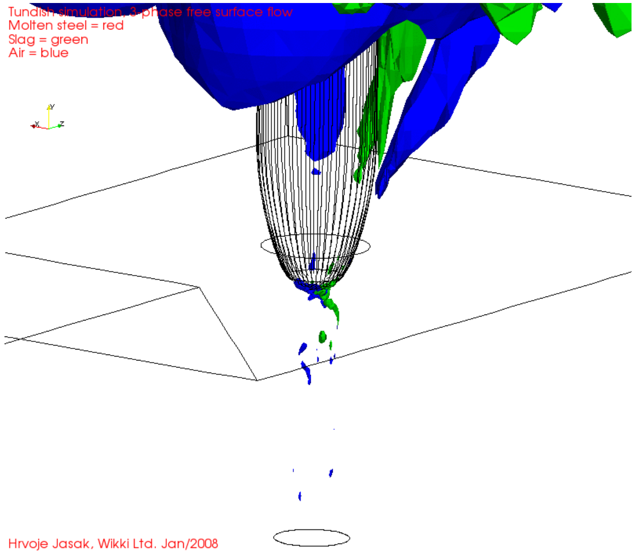
- Injection of Diesel fuel into the atmosphere and subsequent breakup
- $d = 0.2\mathrm{mm}$, high velocity and surface tension
- Mean injection velocity: $460\mathrm{m/s}$ injected into air, $5.2\mathrm{MPa}$, $900\mathrm{K}$
- 1.2 to 8 million cells, aggressive local mesh refinement
- 50k time-steps, $6\mu\mathrm{s}$ initiation time, $20\mu\mathrm{s}$ averaging time



Free Surface Flow Model

Examples: Three-Phase Free Surface Flow in a Tundish

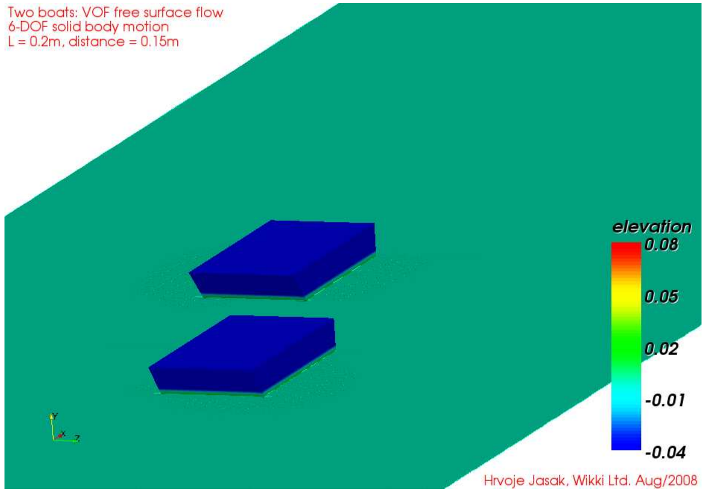
- 3 phases with extreme density ratio: liquid steel, liquid slag, air (7000:2500:1)
- Similar viscosity ratio, probably requires a temperature-dependent model
- Note the presence of multiple phase-to-phase interfaces: using consistent discretisation across phase γ equations
- Simultaneous filling and pouring with large outlet velocity
- Temperature-dependent properties of slag and steel

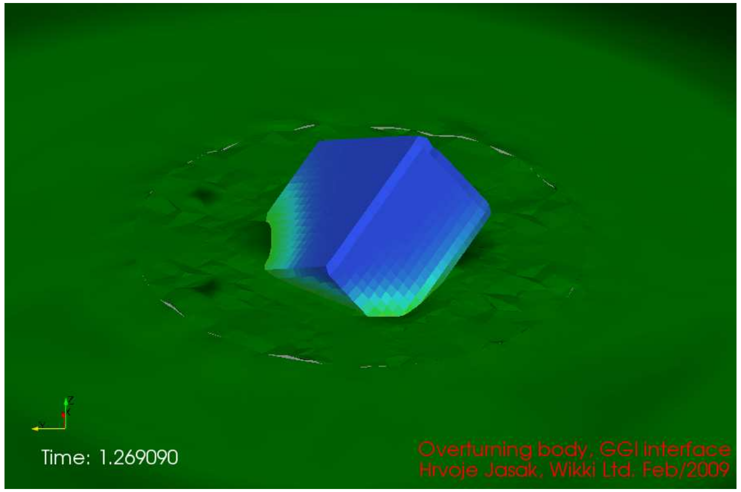


Free Surface Flow Model

Examples: Floating Body

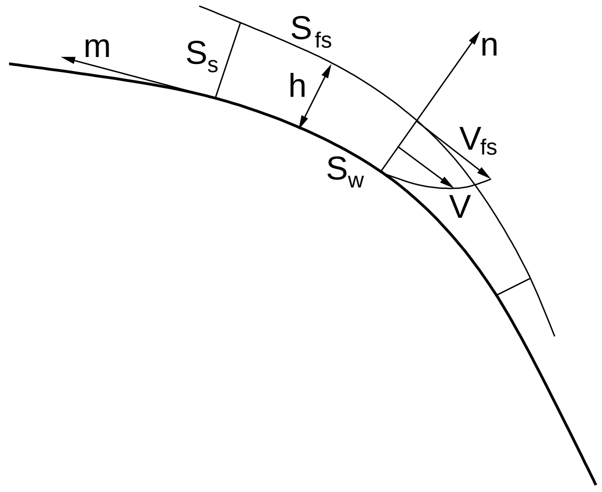
- Combining the 6-Degrees-of-Freedom (6-DOF) solid body motion solver with automatic moving mesh and free surface flow solver
- Floating body is considered rigid and supported by fluid forces: buoyancy
- Integration of 6-DOF solver for translation and rotation of the body
- Surface force calculation integrated in the solver: pressure + skin friction
- Automatic mesh motion adjusts body position dynamically during the run: elastic deformation can be added trivially
- Moving mesh formulation of free surface VOF uses dynamic mesh capability





Liquid Film Model

- Model developed for cases of thin film, where film thickness is small compared to other geometrical dimensions
- Equations are derived prescribing a velocity profile across film thickness and integrating conservation equations over the film



- Working variables
  - Film thickness h, derived from mass conservation and handling pressure
  - Mean film velocity $\mathbf{V}$
- Equation set solved in 2-D, accounting for gravity, surface tension and surface curvature; shear stress on the wall and free surface of liquid film are taken into account as area-based terms

Liquid Film Model

Equation Set of a This Liquid Film Model

- Continuity equation

$$\frac{\partial h}{\partial t} + \nabla_s \bullet (\bar{\mathbf{v}} h) = \frac{\dot{m}_S}{\rho_L};$$

- Momentum equation

$$\frac{\partial (h\bar{\mathbf{v}})}{\partial t} + \nabla_s \bullet (h\bar{\mathbf{v}}\bar{\mathbf{v}} + \mathbf{C}) = \frac{1}{\rho_L}\left(\boldsymbol{\tau}_{fs} - \boldsymbol{\tau}_w\right) + h\mathbf{g}_t - \frac{h}{\rho_L}\nabla_s p_L + \frac{1}{\rho_L}\bar{\mathbf{S}}_v;$$

- Shear stress terms and the convection term correction tensor $\mathbf{C}$ are calculated from prescribed velocity profile
- Liquid film pressure

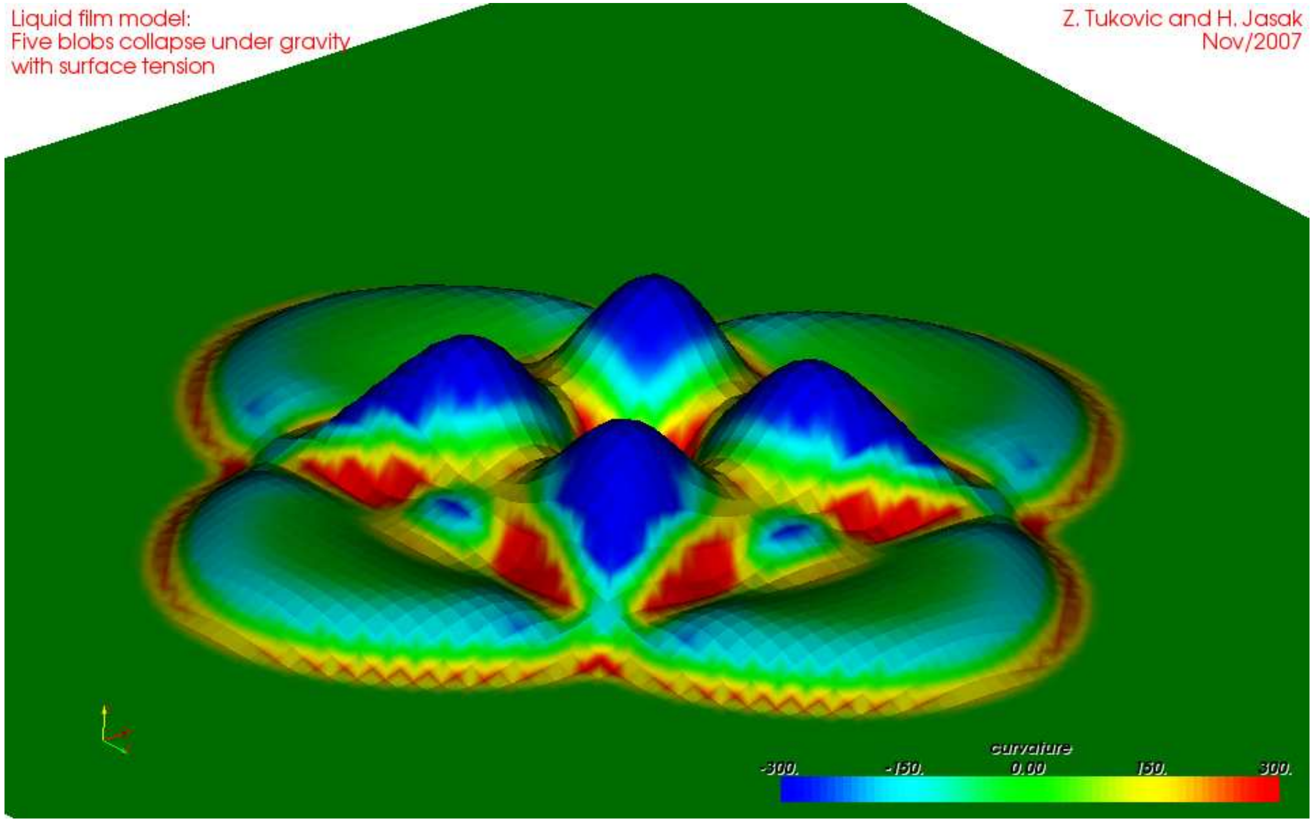
$$p_L = p_g + p_d + p_\sigma + p_h$$

  where
  - p_g is the gas pressure
  - p_d is the droplet impact pressure
  - p_σ is capillary (or Laplace) pressure
  - p_h is hydrostatic pressure

Liquid Film Model

Solution of Surface-Based Equations: Finite Area Method

- Liquid film model: shallow water model on a curved surface with surface tension
- Mesh organisation attached to volumetric FVM solver: easy coupling between surface discretisation and flow equations
- Example: collapse of five surface blobs under surface tension and gravity



Lagrangian Particle Tracking

Integration of Discrete Phase Equations

- Momentum equation for a single droplet in Lagrangian frame

$$m_d \frac{d\mathbf{u}_d}{dt} = \mathbf{F}_d + \mathbf{F}_p + \mathbf{F}_v + \mathbf{F}_b$$

  - $\mathbf{F}_d$ is the drag force:

$$\mathbf{F}_d = \frac{1}{2} C_d \rho A_d \mathbf{u}_{rel} |\mathbf{u}_{rel}|$$

  - $\mathbf{F}_p$ is the pressure force:

$$\mathbf{F}_p = -V_d \nabla p$$

  - $\mathbf{F}_v$ is the virtual mass force:

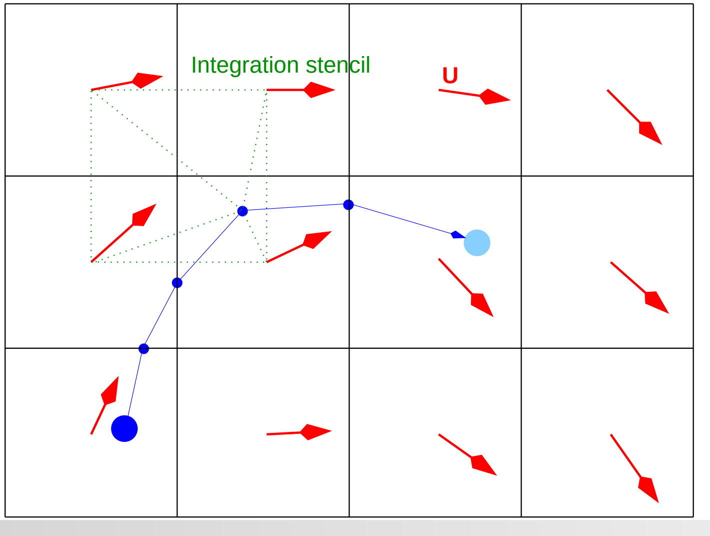
$$\mathbf{F}_v = -C_a \rho V_d \frac{d\mathbf{u}_{rel}}{dt}$$

  - $\mathbf{F}_b$ is the body force, e.g. gravity
- Droplet position is integrated by tracking: $\frac{d\mathbf{x}_d}{dt} = \mathbf{u}_d$

Lagrangian Particle Tracking

Integration of Motion Equation

- Motion equation for a particle is an Ordinary Differential Equation (ODE)
- During integration, particle traverses a number of cells and continuous phase properties are updated based on its position
- For accurate integration, motion equation is formulated as an ODE and solver using an ODE solver
- Additional physics can be attached to the particle, eg. chemistry, evaporation, turbulence interaction
- If more accurate integration is necessary, sub-cycling may be implemented: particle time-step depends on min physics time-scale



Lagrangian Particle Tracking

Euler-Lagrange Multi-Phase Model

- Continuous phase represented by Euler equations, assuming low volume fraction of the dispersed phase ($< 10\%$)
- Dispersed phase modelled by tracking particles in a mesh, with momentum exchange between the two
- In continuous phase equations it is assumed that the dispersed phase is sufficiently dilute to neglect dispersed phase volume fraction effects
- Coupling appears in the continuous momentum equation:

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla\bullet(\mathbf{u}\mathbf{u}) - \nabla\bullet\boldsymbol{\sigma} = -\nabla p + \mathbf{s}_{ud}$$

- $\mathbf{s}_{ud}$ is the total momentum exchange between the continuous and discrete phase. This is calculated on a per-cell basis:

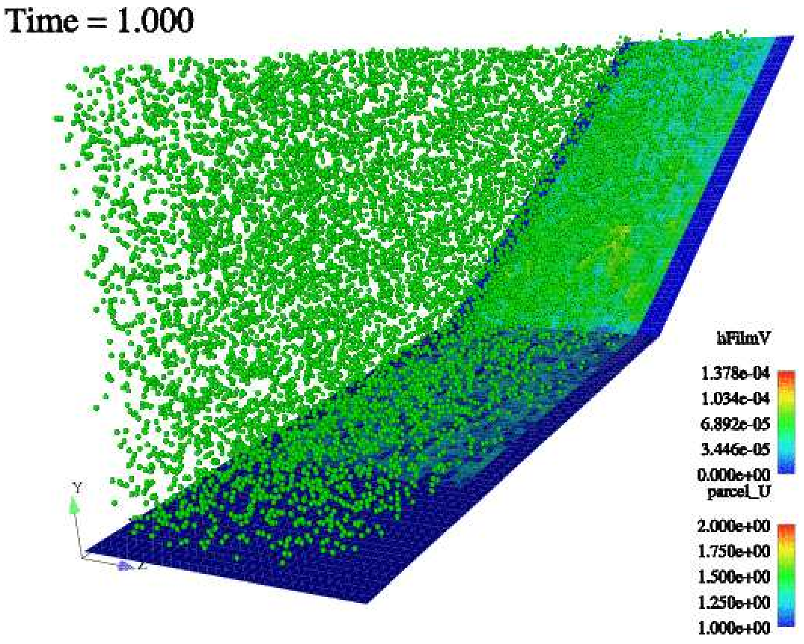
$$\mathbf{s}_{ud} = \frac{1}{V} \sum_{\text{d in V}} \left[m_d \frac{\mathbf{u}_d - \mathbf{u}_d^o}{\Delta t} - \mathbf{F}_p - \mathbf{F}_b \right]$$

- Effective viscosity and source/sink term volume correction is also used

Lagrangian Particle Tracking

Vehicle Soling Simulation: Coupled Eulerian, Lagrangian and Wall Transport Model

- Continuous phase: external aerodynamics flow model; coupled or uncoupled
- Lagrangian tracking for droplets: drag, pressure term, gravity
- Liquid film model capturing surface transport
- Coupling between components depends on the objective of the simulation. Potentially, all components are coupled, but in some cases this can safely be ignored



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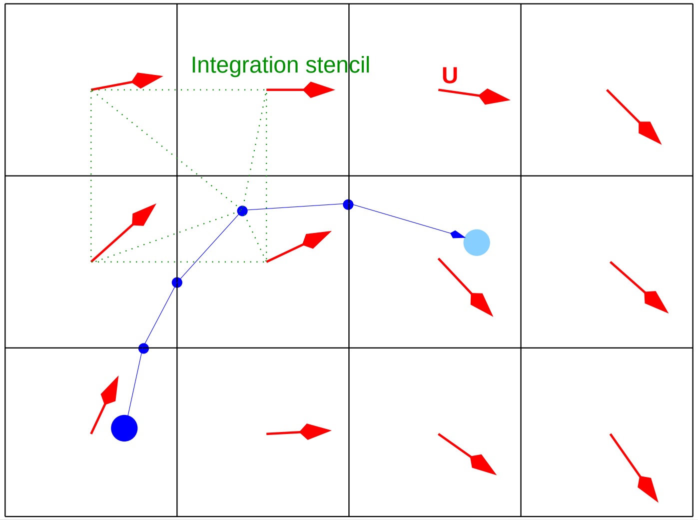


Free Surface Tracking

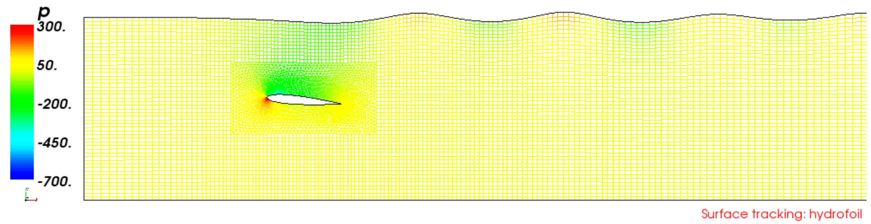
Free Surface Tracking Simulations

- A free surface flow system can be viewed as two sets of fluid flow equations coupled at the surface. Surface conditions:
  - Free surface is infinitely thin
  - There is no flow through the free surface: fluids are separated
  - **Kinematic condition**: Normal velocity component must be continuous across the interface
  - **Dynamic condition**: Forces acting on the fluid at the interface are in equilibrium
- In practice, motion of one side and pressure from the other side will be exchanged until both conditions are satisfied
- Free surface tracking may be interpreted as a FV simulation on a moving deforming mesh, where the position of the free surface is a part of the solution and not known in advance
- In practical simulations, only the surface deformation is known: the rest of the mesh must accommodate boundary motion

Free Surface Tracking

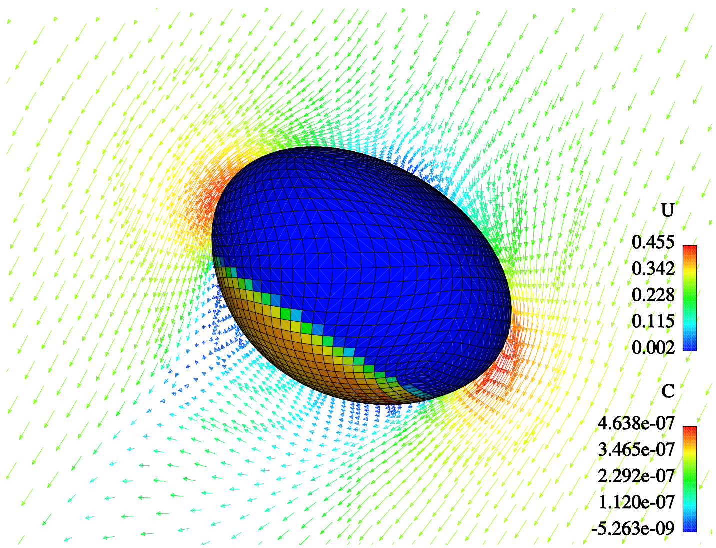
Hydrofoil Under A Free Surface

- Flow solver gives surface displacement
- Mesh adjusted to free surface position



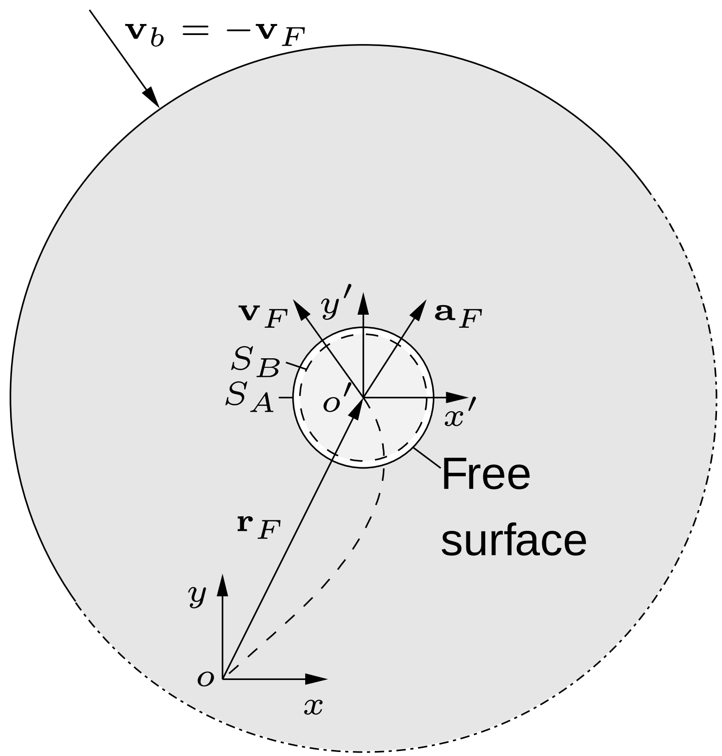
Free-Rising Air Bubble with Surfactants

- Two meshes coupled on free surface



Single Solver, Complex Coupling

- FVM on moving meshes
- Automatic mesh motion
- FAM: Surface physics



Summary

Multiphase Flow Modelling

- Eulerian multi-phase model for inter-penetrating continua
- In cases where the characteristic size of dispersed phase is a part of the solution, population balance modelling needs to be included
- Free surface VOF solver: volumetric surface capturing
- Lagrangian particle tracking: discrete particle model
- Free surface tracking model: mesh motion adheres to free surface position