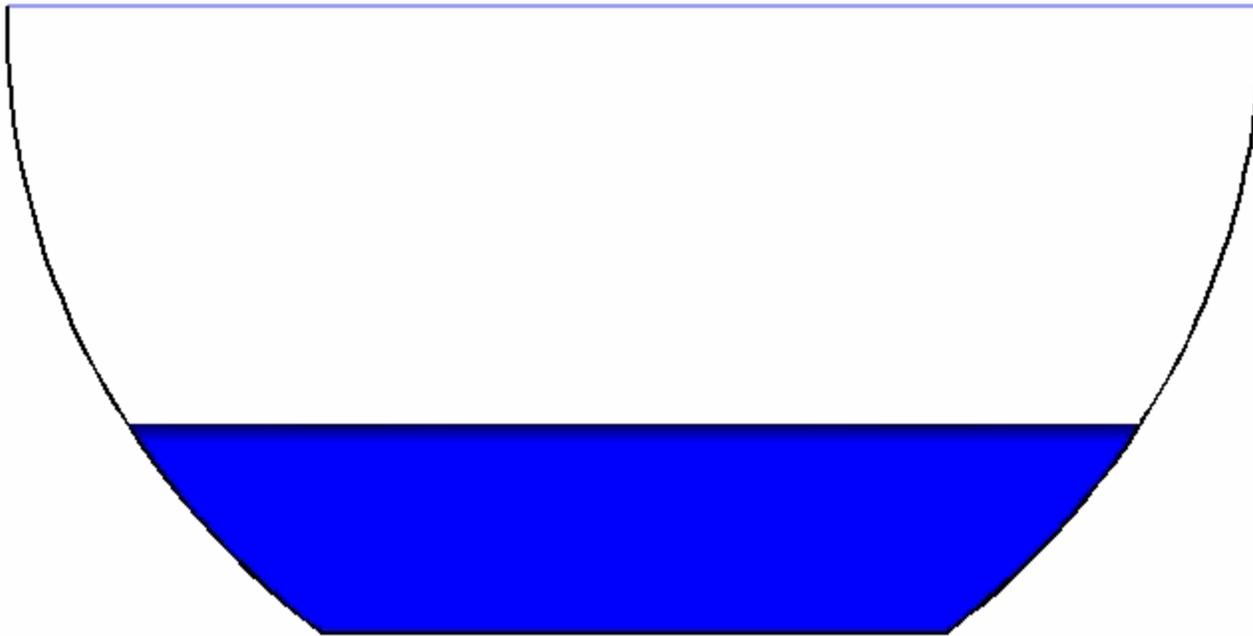# Lecture 16 - Free Surface Flows
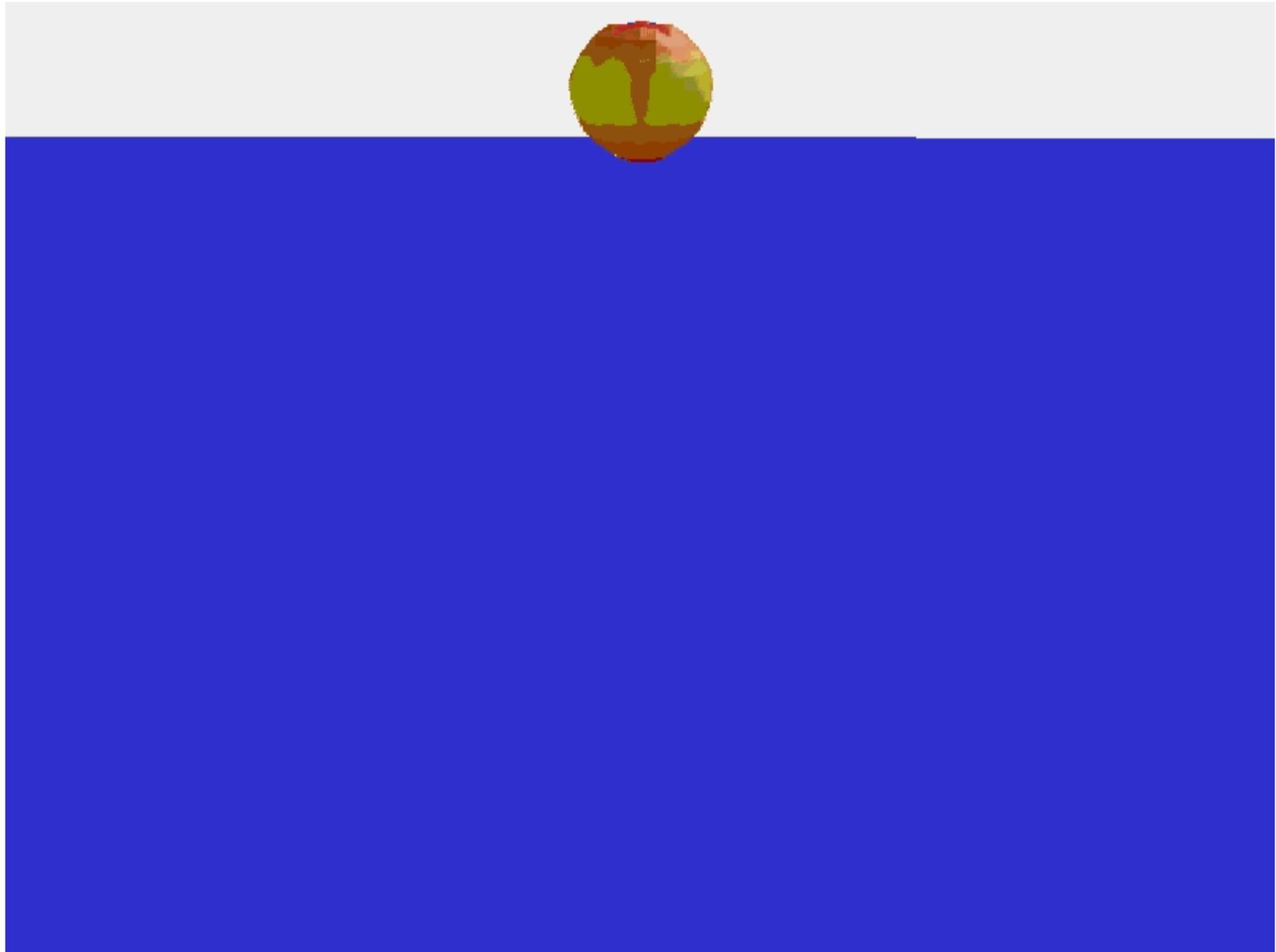
Applied Computational Fluid Dynamics

Instructor: André Bakker

Example: spinning bowl

- Example: flow in a spinning bowl.
- Re = 1E6
- At startup, the bowl is partially filled with water. The water surface deforms once the bowl starts spinning. The animation covers three full revolutions.

Example: splashing droplet

Example: pouring water

- A bucket of water is poured through the air into a container of kerosene.

- This disrupts the kerosene, and air bubbles formed soon rise to the surface and break.

- The three liquids in this simulation do not mix, and after a time the water collects at the bottom of the container.

- The sliding mesh model is used to model the tipping of the bucket.
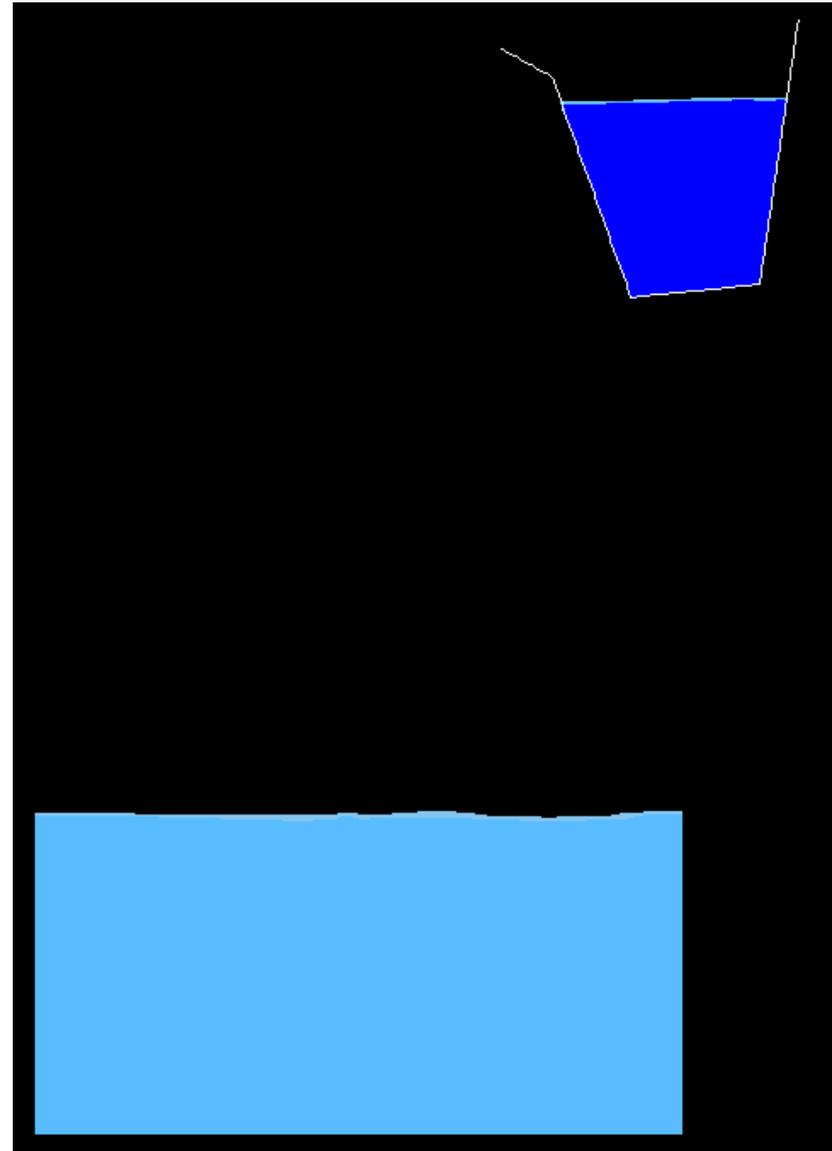
VOF Model

- Volume of fluid (VOF) model overview.
- VOF is an Eulerian fixed-grid technique.
- Interface tracking scheme.
- Application: modeling of gravity current.
- Surface tension and wall adhesion.
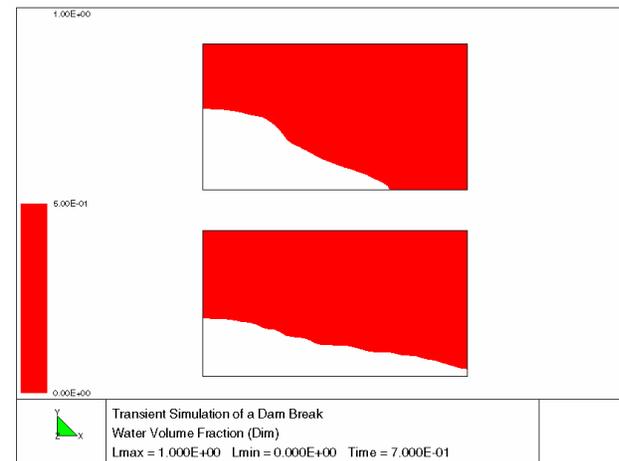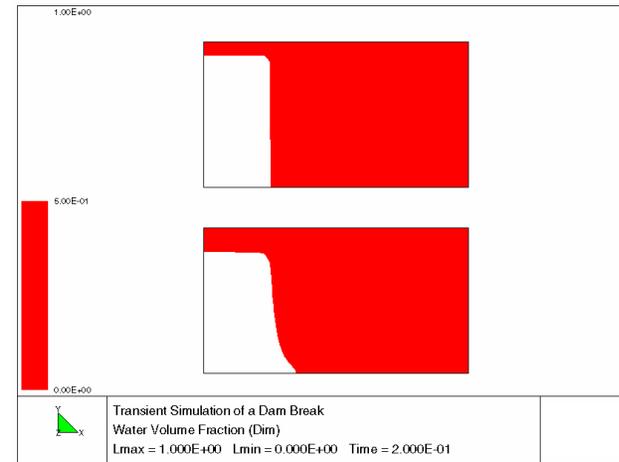- Solution strategies.
- Summary.
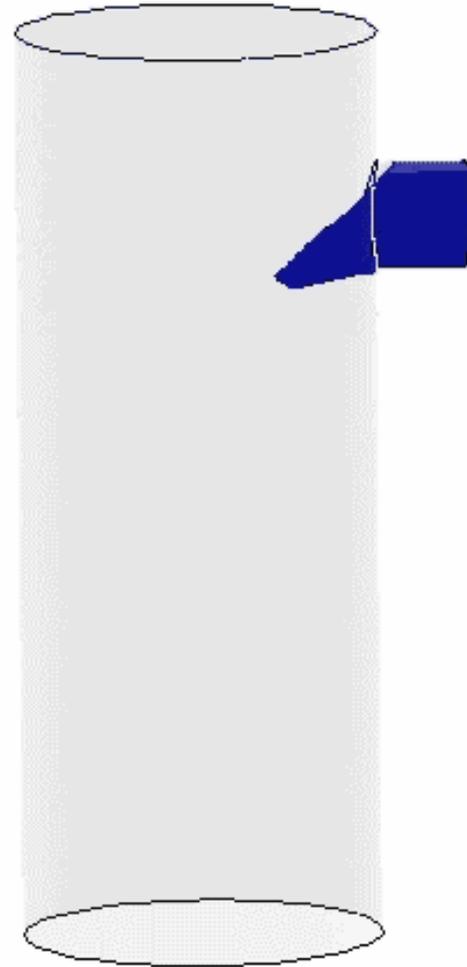
Modeling techniques

- Lagrangian methods:
  - The grid moves and follows the shape of the interface.
  - Interface is specifically delineated and precisely followed.
  - Suited for viscous, laminar flows.
  - Problems of mesh distortion, resulting in instability and internal inaccuracy.
- Eulerian methods:
  - Fluid travels between cells of the fixed mesh and there is no problem with mesh distortion.
  - Adaptive grid techniques.
  - Fixed grid techniques, e.g. volume of fluid (VOF) method.
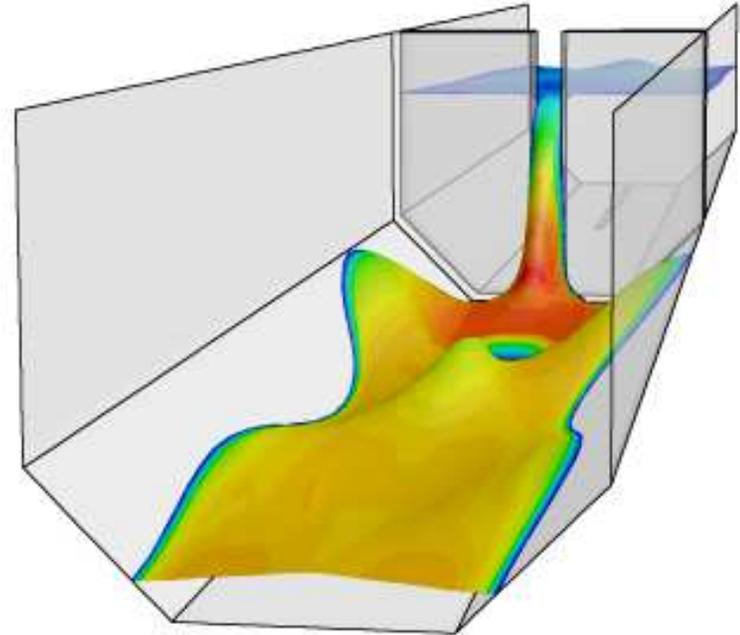
Volume of fluid model

- Immiscible fluids with clearly defined interface.
  - Shape of the interface is of interest.
- Typical problems:
  - Jet breakup.
  - Motion of large bubbles in a liquid.
  - Motion of liquid after a dam break.
  - Steady or transient tracking of any liquid-gas interface.
- Inappropriate if bubbles are small compared to a control volume (bubble columns).

Transient Simulation of a Dam Break
Water Volume Fraction (Dim)
Lmax = 1.000E+00 Lmin = 0.000E+00 Time = 2.000E-01

Transient Simulation of a Dam Break
Water Volume Fraction (Dim)
Lmax = 1.000E+00 Lmin = 0.000E+00 Time = 7.000E-01

VOF

- Assumes that each control volume contains just one phase (or the interface between phases).
- Solves one set of momentum equations for all fluids.

$$\frac{\partial}{\partial t}(\rho u_j) + \frac{\partial}{\partial x_i}(\rho u_i u_j) = -\frac{\partial P}{\partial x_j} + \frac{\partial}{\partial x_i}\mu(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}) + \rho g_j + F_j$$

- Surface tension and wall adhesion modeled with an additional source term in momentum equation.
- For turbulent flows, single set of turbulence transport equations solved.
- Solves a volume fraction conservation equation for the secondary phase.

Volume fraction

- Defines a step function ε equal to unity at any point occupied by fluid and zero elsewhere such that:

$$\varepsilon_k\left(cell\right) = \frac{\iiint\limits_{cell} \varepsilon_k(x, y, z)dxdydz}{\iiint\limits_{cell} dxdydz}$$

- For volume fraction of kth fluid, three conditions are possible:
  - $\varepsilon_k = 0$ if cell is empty (of the kth fluid).
  - $\varepsilon_k = 1$ if cell is full (of the kth fluid).
  - $0 < \varepsilon_k < 1$ if cell contains the interface between the fluids.
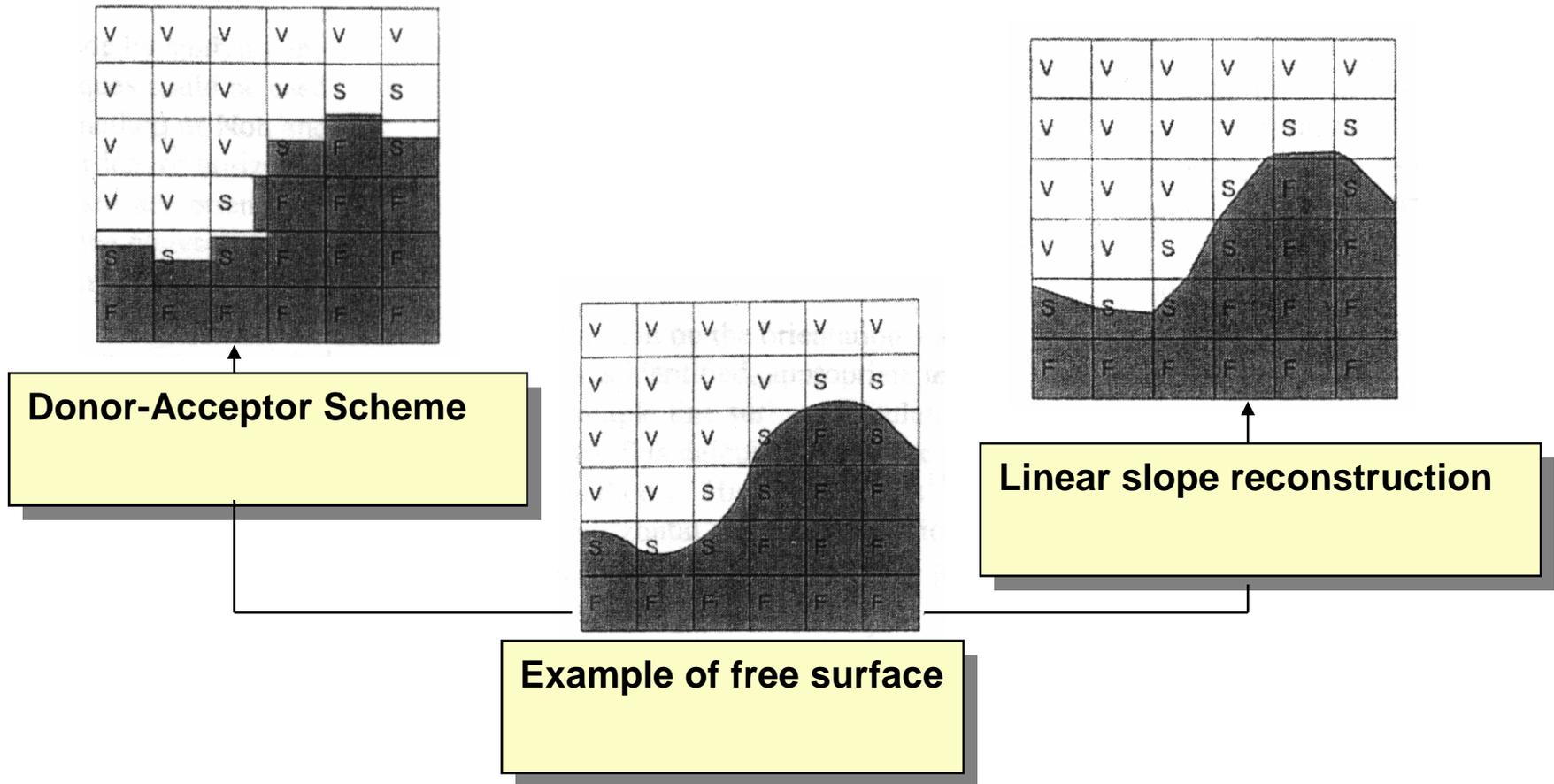
Volume fraction (2)

- Tracking of interface(s) between phases is accomplished by solution of a volume fraction continuity equation for each phase:

$$\frac{\partial \varepsilon_k}{\partial t} + u_j \frac{\partial \varepsilon_k}{\partial x_i} = S_{\varepsilon_k}$$

- Mass transfer between phases can be modeled by using a user-defined subroutine to specify a nonzero value for $S_{\varepsilon k.}$

- Multiple interfaces can be simulated.

- Cannot resolve details of the interface smaller than the mesh size.

Interface tracking schemes

Donor-Acceptor Scheme

Example of free surface

Linear slope reconstruction
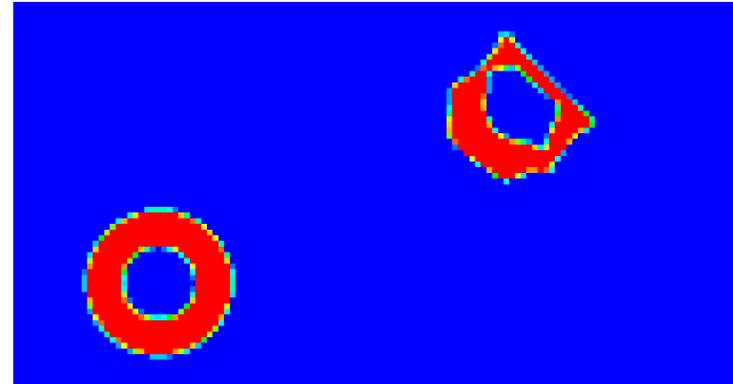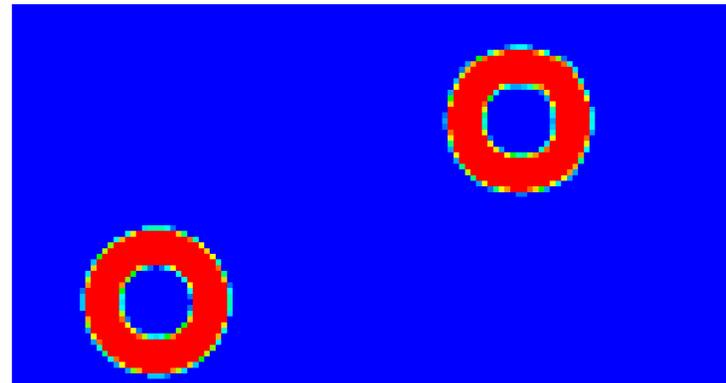
Comparing different interface tracking schemes
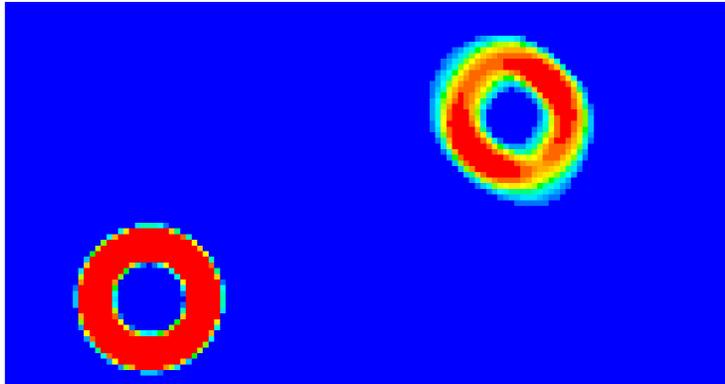
2nd order upwind. Interface is not tracked explicitly. Only a volume fraction is calculated for each cell.


Donor - Acceptor


Geometric reconstruction

Surface tension

- Surface tension along an interface arises from attractive forces between molecules in a fluid (cohesion).

- Near the interface, the net force is radially inward. Surface contracts and pressure increases on the concave side.

- At equilibrium, the opposing pressure gradient and cohesive forces balance to form spherical bubbles or droplets.
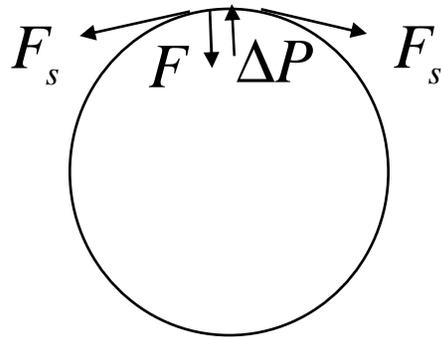
$$\Delta P = \sigma \left(\frac{1}{R_1} + \frac{1}{R_2} \right)$$

Surface tension example

- Cylinder of water (5 x 1 cm) is surrounded by air in no gravity.
- Surface is initially perturbed so that the diameter is 5% larger on ends.
- The disturbance at the surface grows by surface tension.
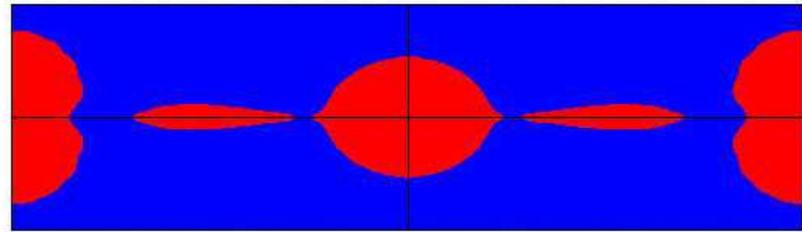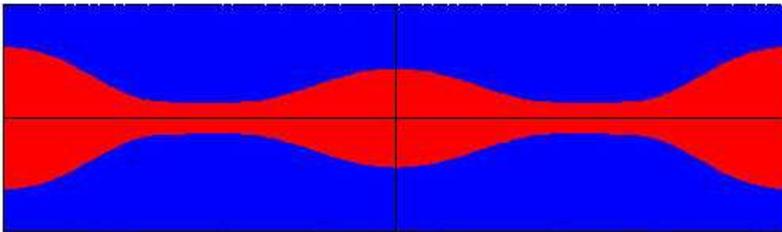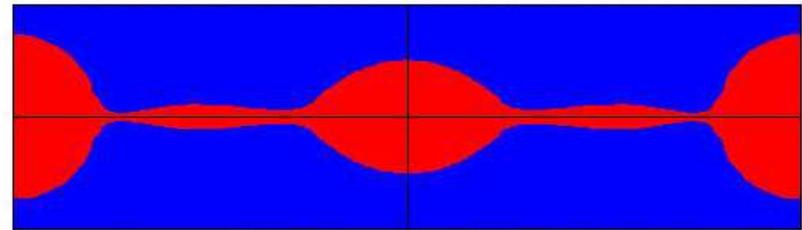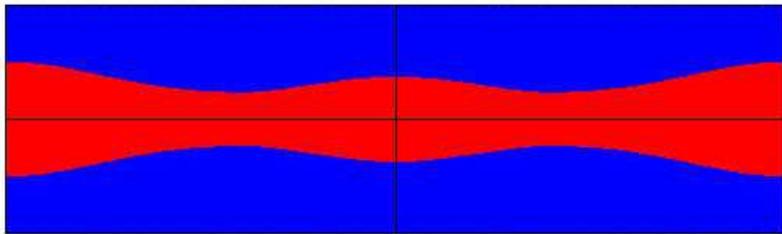
Surface tension - when important

- To determine significance, first evaluate the Reynolds number.

$$Re = \frac{\rho UL}{\mu}$$

- For Re << 1, evaluate the Capillary number.

$$Ca = \frac{\mu U}{\sigma}$$

- For Re >> 1, evaluate the Weber number.

$$We = \frac{\sigma}{\rho LU^2}$$

- Surface tension important when We >>1 or Ca<< 1.
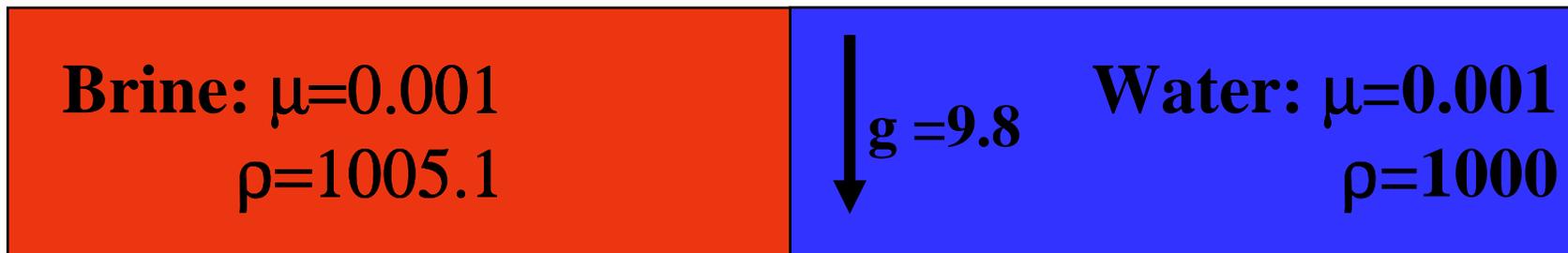- Surface tension modeled with an additional source term in momentum equation.

Wall adhesion

- Large contact angle (> 90°) is applied to water at bottom of container in zero-gravity field.

- An obtuse angle, as measured in water, will form at walls.

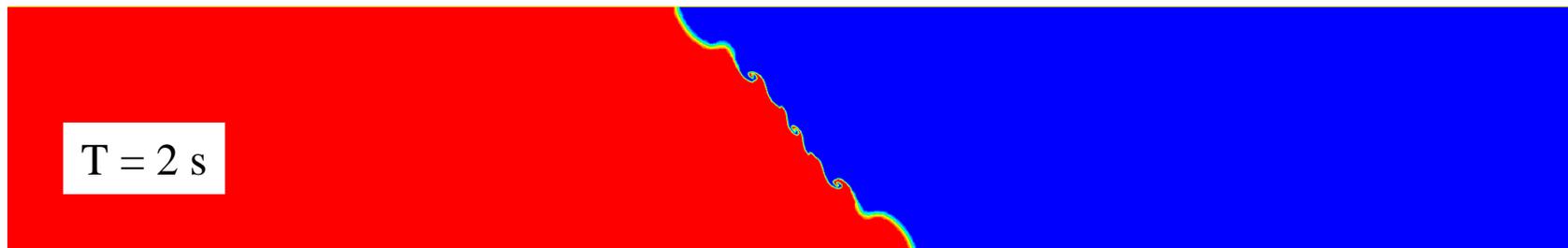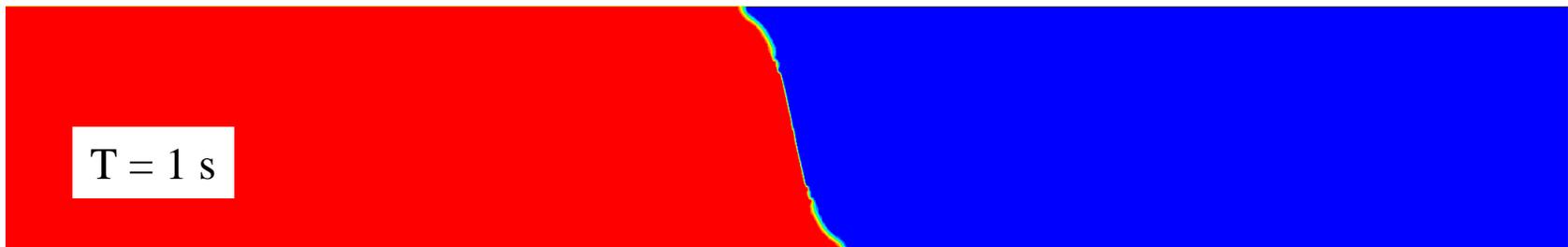- As water tries to satisfy contact angle condition, it detaches from bottom and moves slowly upward, forming a bubble.
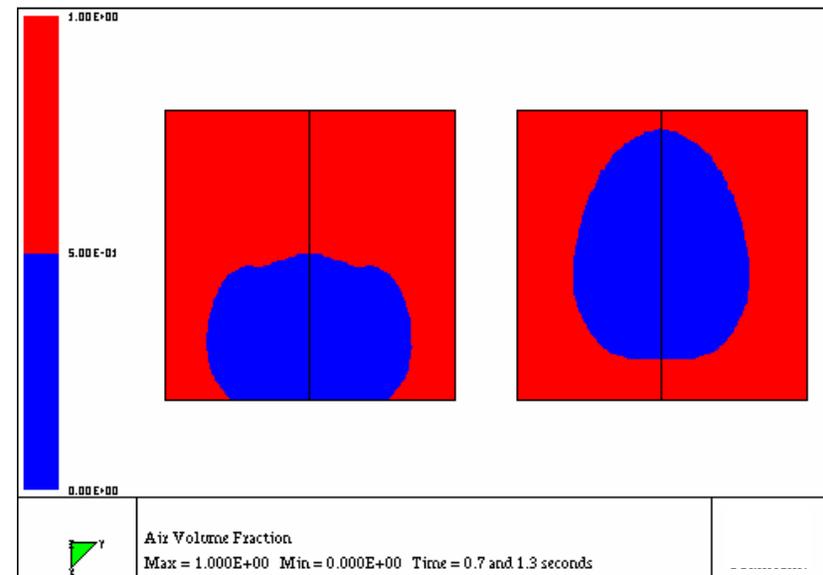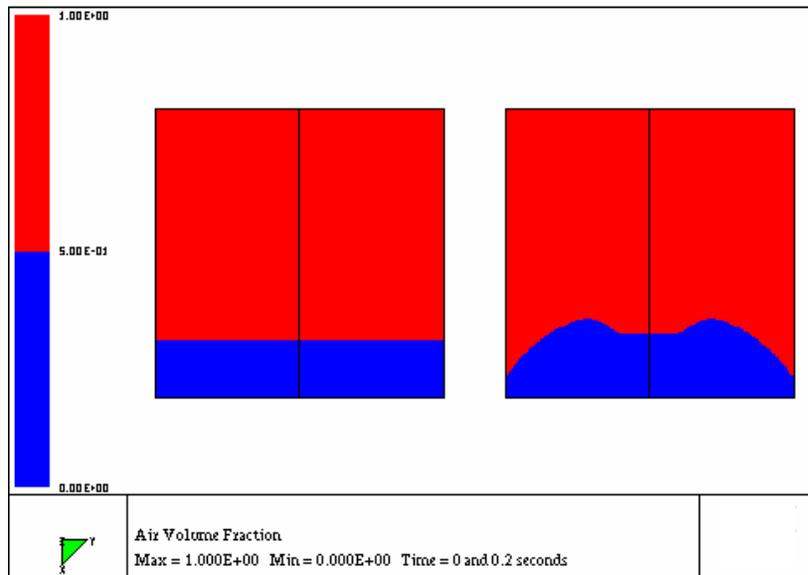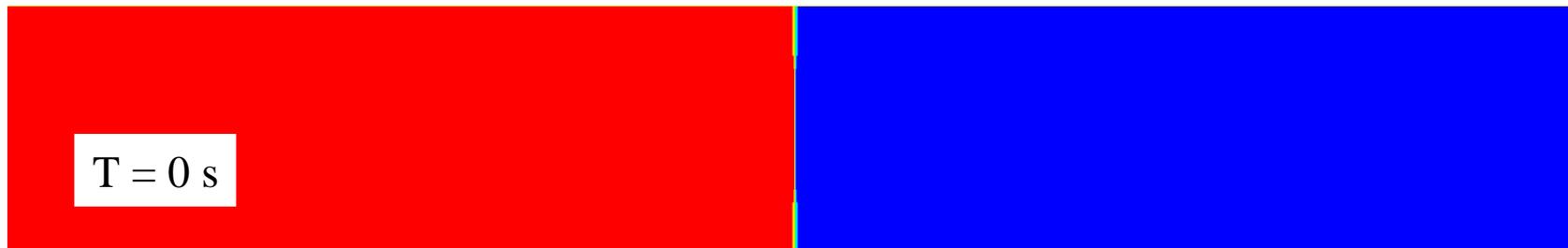
Modeling of the gravity current

- Mixing of brine and fresh water.
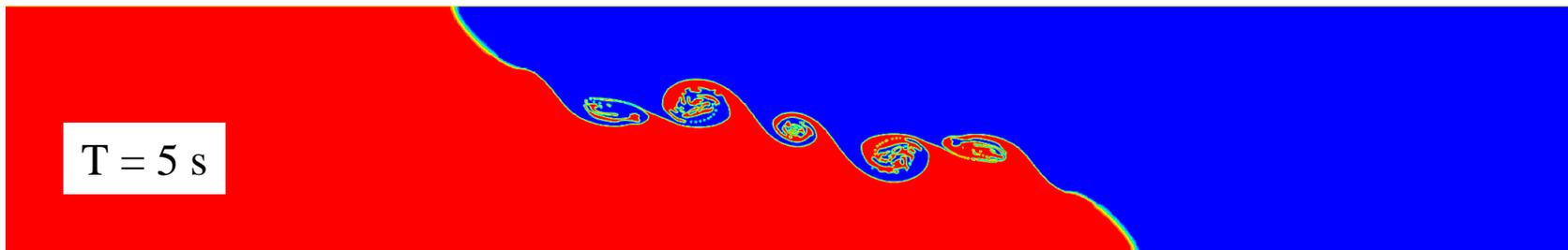   - 190K cells with hanging nodes.
    - Domain: length 1m, height 0.15m.
    - Time step: 0.002 s.
    - PISO algorithm.
    - Geometric reconstruction scheme.
    - QUICK scheme for momentum.
    - Run time ~8h on an eight-processor (Ultra2300) network.

Brine: μ=0.001 ρ=1005.1

g =9.8

Water: μ=0.001 ρ=**1000**

Gravity current (1)

T = 0 s

T = 1 s

T = 2 s

Gravity current (2)

T = 3 s

T = 4 s

T = 5 s

Gravity current (3)

T = 7 s

T = 9 s

T = 10 s
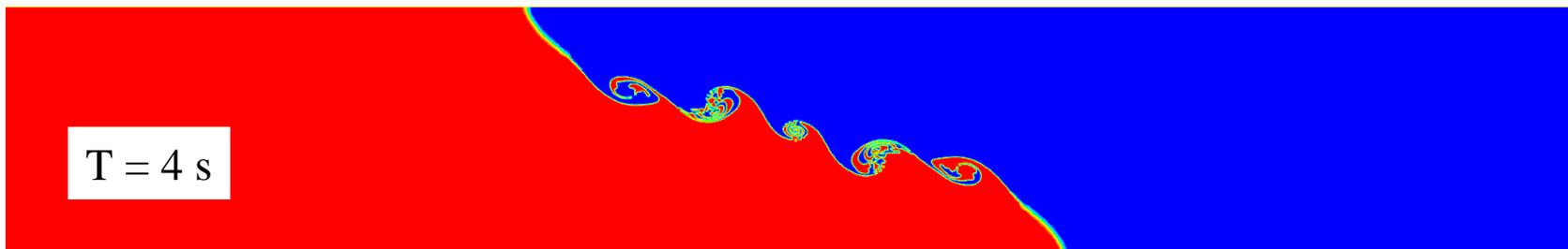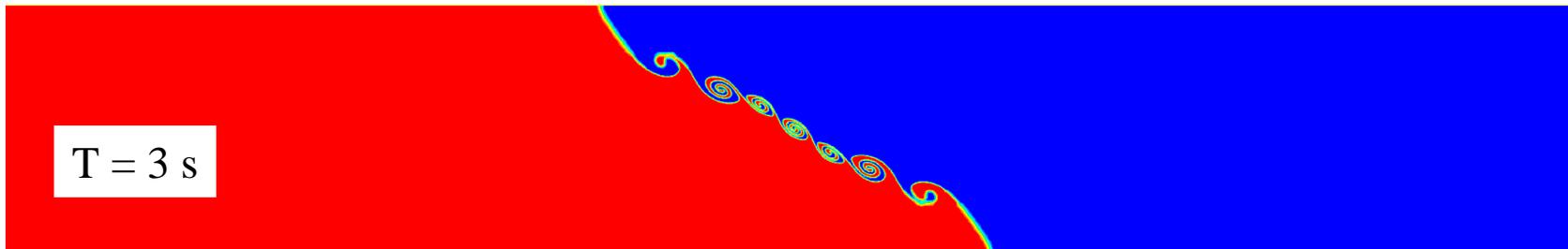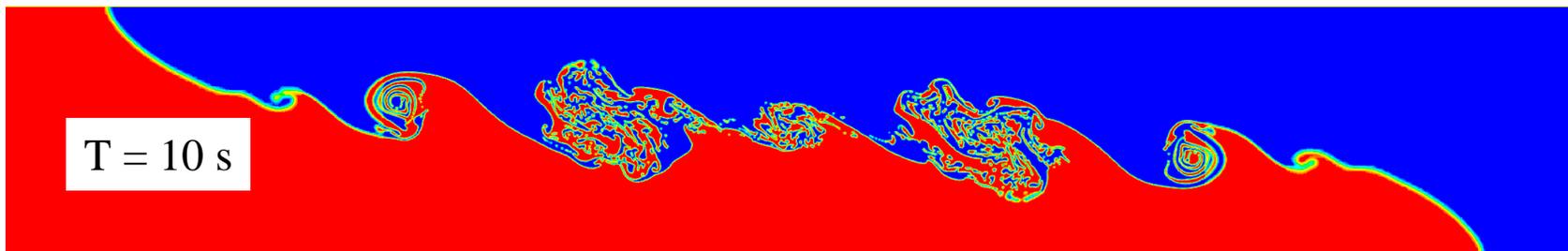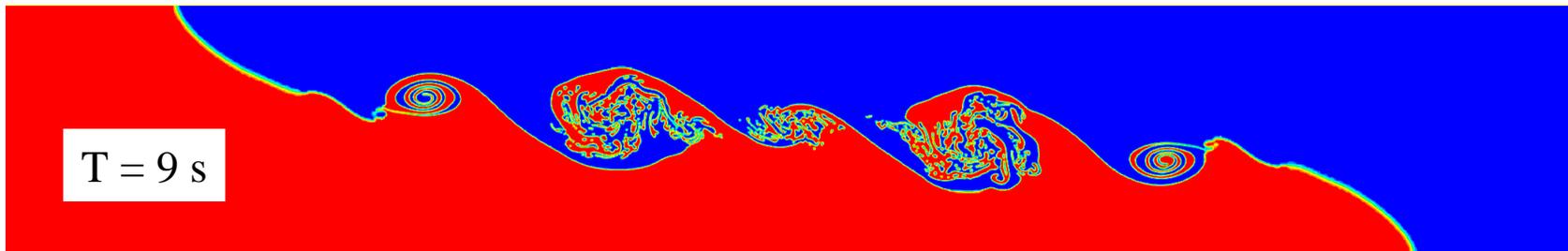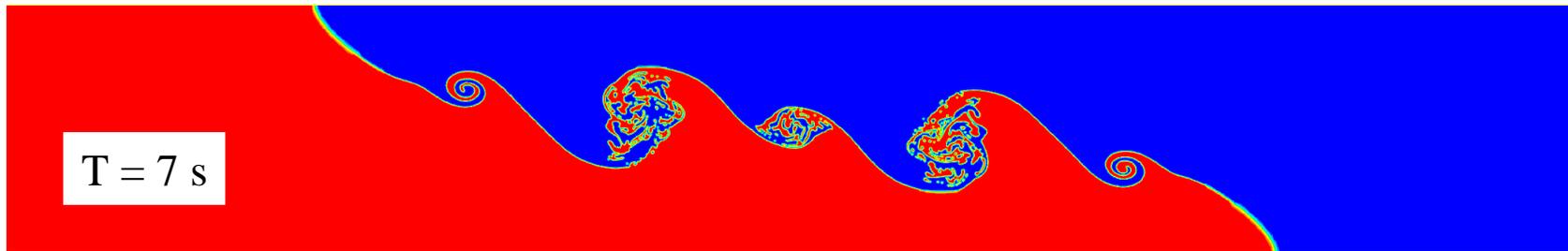
Visco-elastic fluids - Weissenberg effect

- Visco-elastic fluids, such as dough and certain polymers, tend to climb up rotating shafts instead of drawing down a vortex.

- This is called the Weissenberg effect and is very difficult to model.

- The photograph shows the flow of a solution of polyisobutylene.
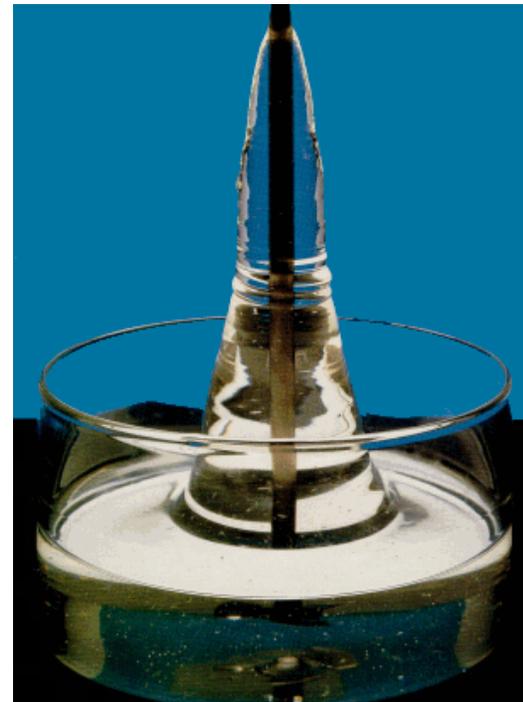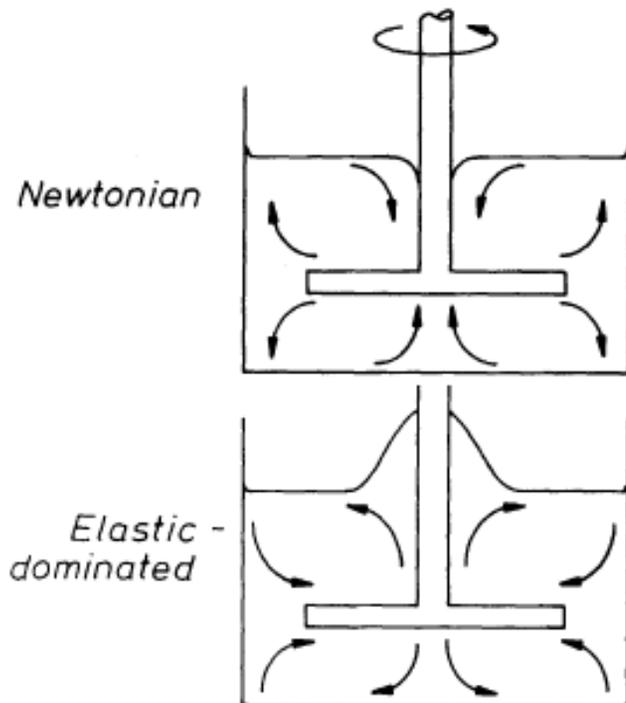
Visco-elastic fluids - blow molding

- Blow molding is a commonly used technique to manufacture bottles, canisters, and other plastic objects.

- Important parameters to model are local temperature and material thickness.

VOF model formulations - steady state

- Steady-state with implicit scheme:
  - Used to compute steady-state solution using steady-state method.
  - More accurate with higher order discretization scheme.
  - Must have distinct inflow boundary for each phase.
  - Example: flow around ship's hull.
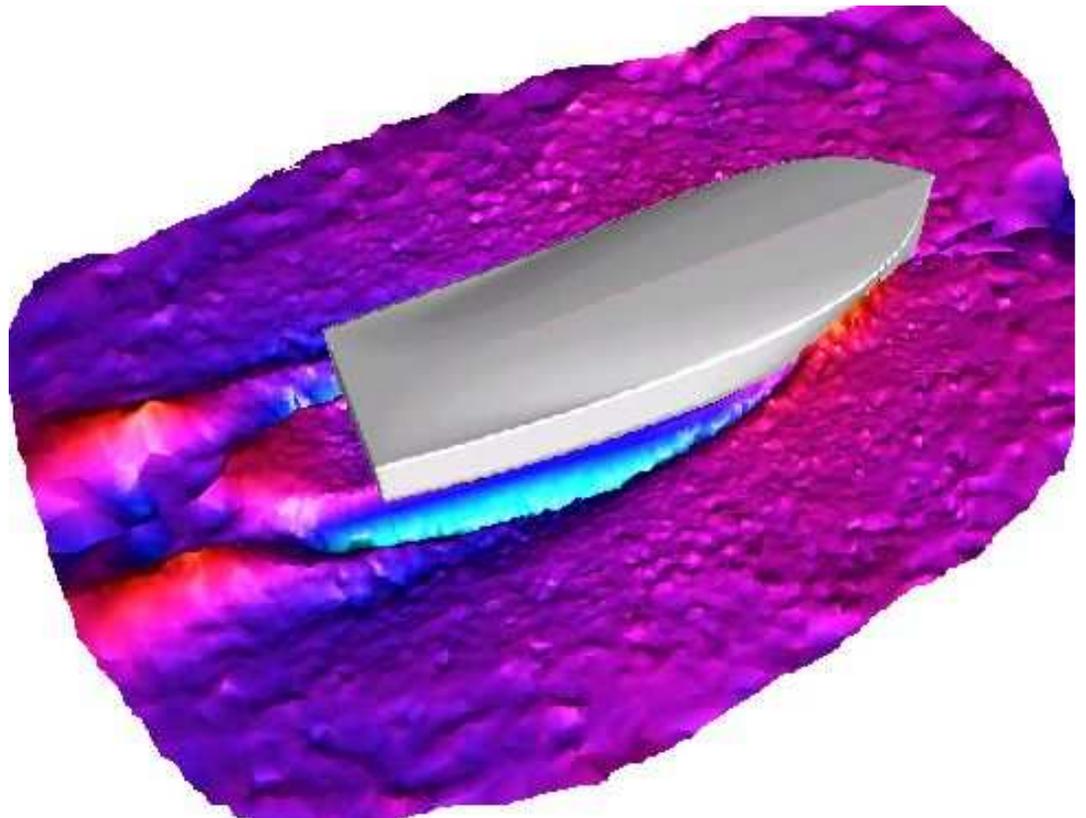
VOF model formulations - time dependent

- Time-dependent with explicit schemes:
  - Use to calculate time accurate solutions.
  - Geometric linear slope reconstruction.
    - Most accurate in general.
  - Donor-acceptor.
    - Best scheme for highly skewed hex mesh.
  - Euler explicit.
    - Use for highly skewed hex cells in hybrid meshes if default scheme fails.
    - Use higher order discretization scheme for more accuracy.
  - Example: jet breakup.

- Time-dependent with implicit scheme:
  - Used to compute steady-state solution when intermediate solution is not important and the final steady-state solution is dependent on initial flow conditions.
  - There is not a distinct inflow boundary for each phase.
  - More accurate with higher order discretization scheme.
  - Example: shape of liquid interface in centrifuge.

VOF solution strategies: time dependence

- Time-stepping for the VOF equation:
  - Automatic refinement of the time step for VOF equation using Courant number C:

$$C = \frac{\Delta t}{\Delta x_{cell} / u_{fluid}}$$

  - Δt is the minimum transit time for any cell near the interface.
- Calculation of VOF for each time-step:
  - Full coupling with momentum and continuity (VOF updated once per iteration within each time-step): more CPU time, less stable.
  - No coupling (default): VOF and properties updated once per time step. Very efficient, more stable but less accurate for very large time steps.

VOF solution strategies (continued)

- To reduce the effect of numerical errors, specify a reference pressure location that is always in the less dense fluid, and (when gravity is on) a reference density equal to the density of the less dense fluid.
- For explicit formulations for best and quick results:
  - Always use geometric reconstruction or donor-acceptor.
  - Use PISO algorithm.
  - Increase all under-relaxation factors up to 1.0.
  - Lower timestep if it does not converge.
  - Ensure good volume conservation: solve pressure correction equation with high accuracy (termination criteria to 0.001 for multigrid solver).
  - Solve VOF once per time-step.
- For implicit formulations:
  - Always use QUICK or second order upwind difference scheme.
  - May increase VOF under-relaxation from 0.2 (default) to 0.5.

Summary

- Free surface flows are encountered in many different applications:
  - Flow around a ship.
  - Blow molding.
  - Extrusion.
  - Mold filling.
- There are two basic ways to model free surface flows:
  - Lagrangian: the mesh follows the interface shape.
  - Eulerian: the mesh is fixed and a local volume fraction is calculated.
- The most common method used in CFD programs based on the finite volume method is the volume-of-fluid (VOF) model.