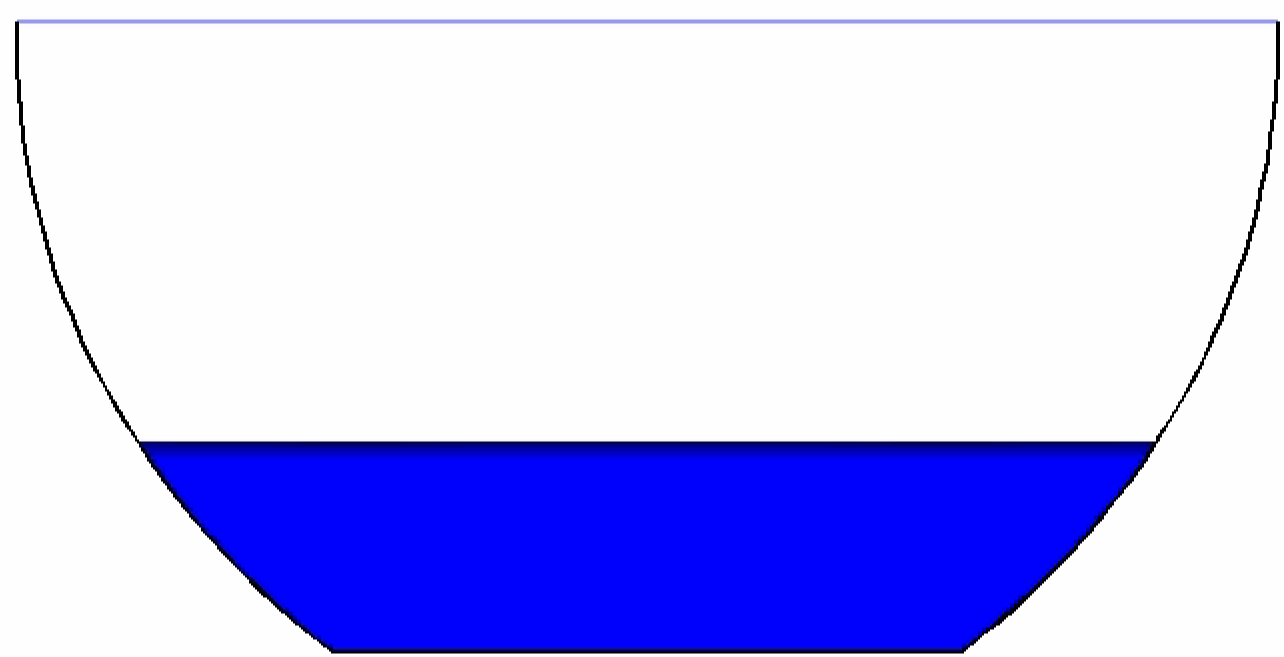
# Lecture 16 - Free Surface Flows

## Applied Computational Fluid Dynamics

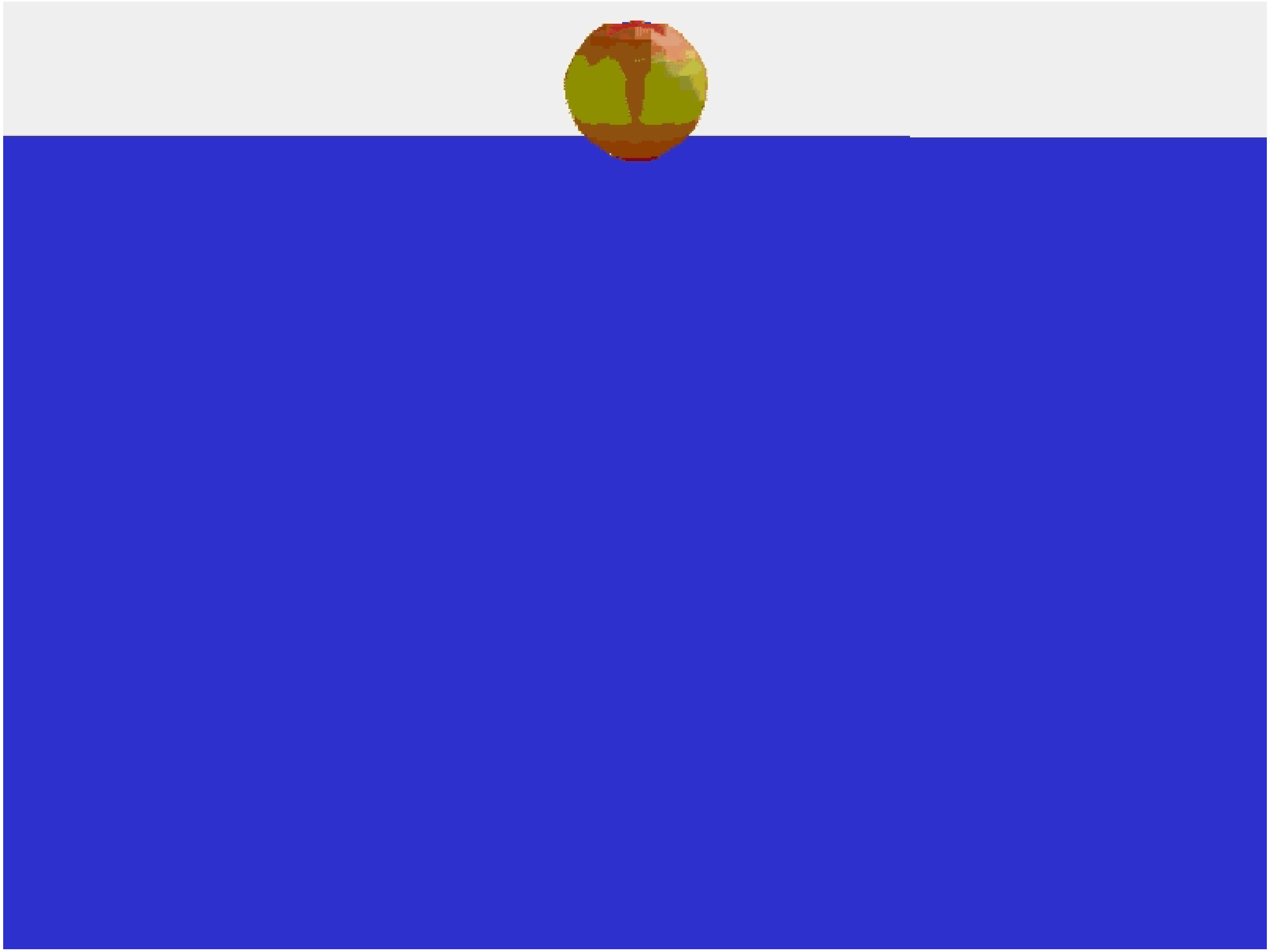
Instructor: André Bakker

# 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.

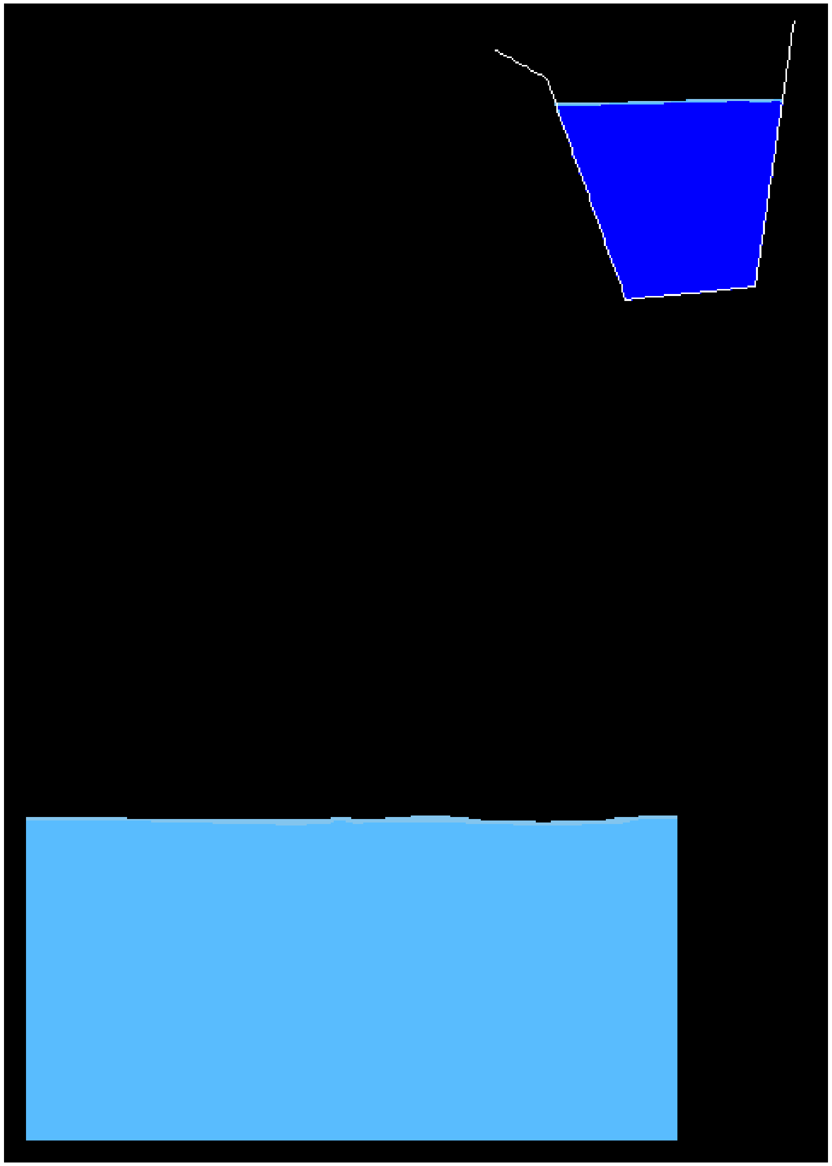


# Example: splashing droplet



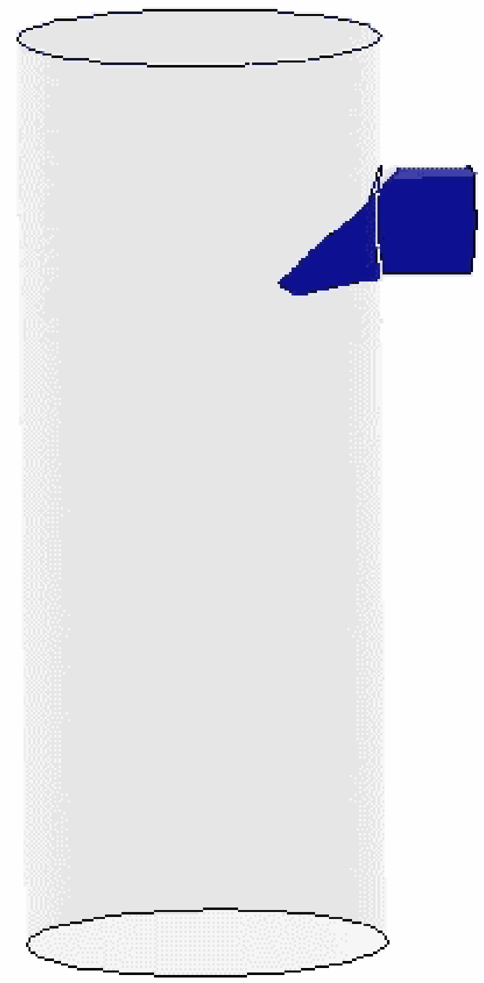
# Example: pouring water

- 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.



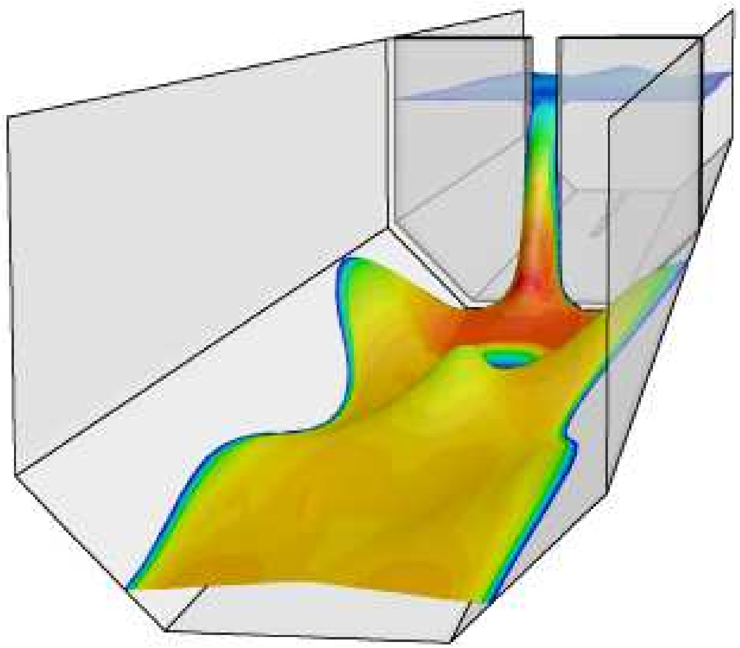
# VOF Model

- 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.



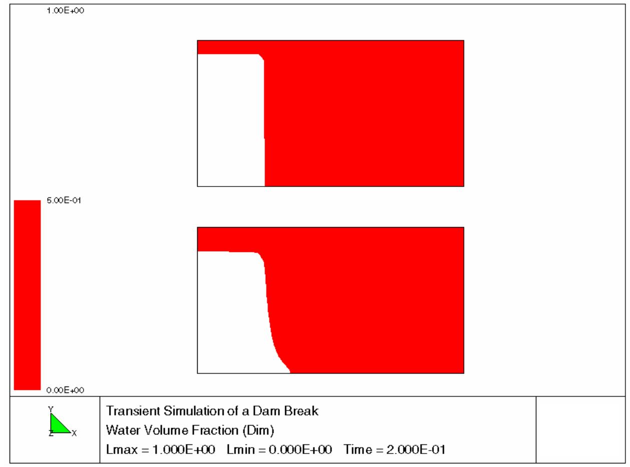
# Modeling techniques

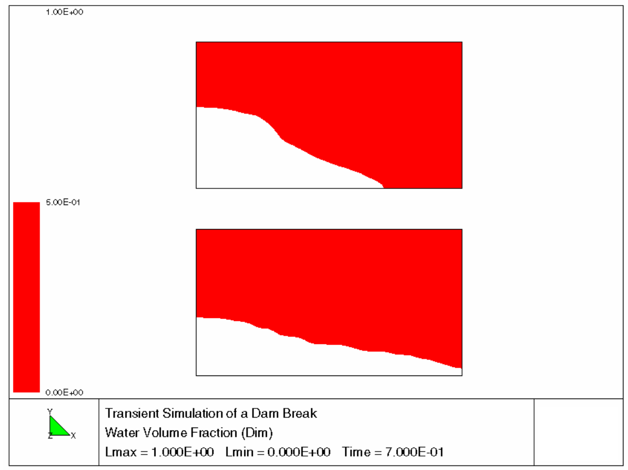
- Lagrangian methods:
  - The grid moves and follows the shape of the interface.
  - Interface is specifically delineated and precisely followed.
  - Suited for viscous, laminar flows.
  - Problems of mesh distortion, resulting in instability and internal inaccuracy.
- Eulerian methods:
  - Fluid travels 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).



# 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 $\varepsilon$ equal to unity at any point occupied by fluid and zero elsewhere such that:

$$\varepsilon_k(cell) = \frac{\iiint_{cell} \varepsilon_k(x, y, z)\,dxdydz}{\iiint_{cell} dxdydz}$$

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

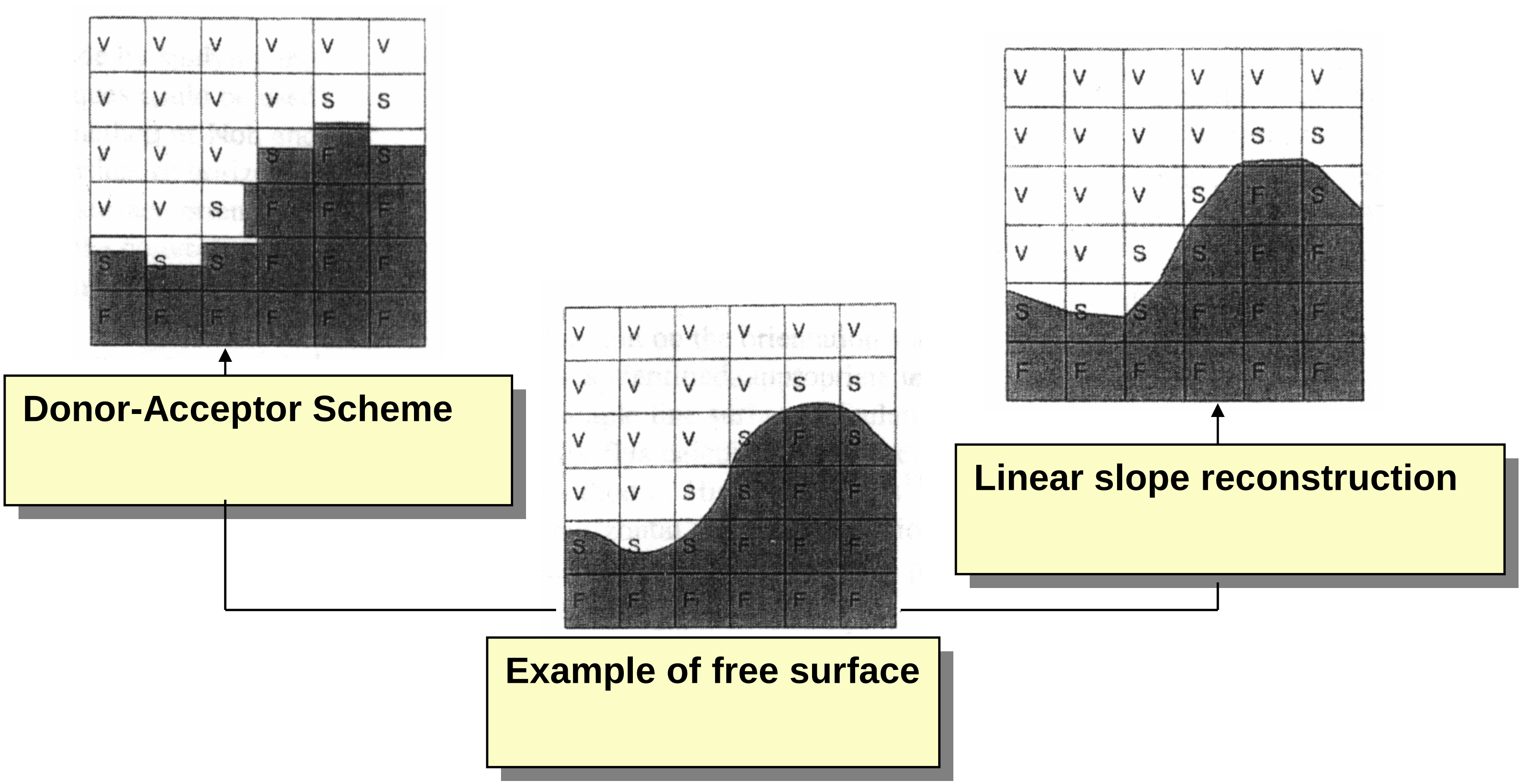
# Volume fraction (2)

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

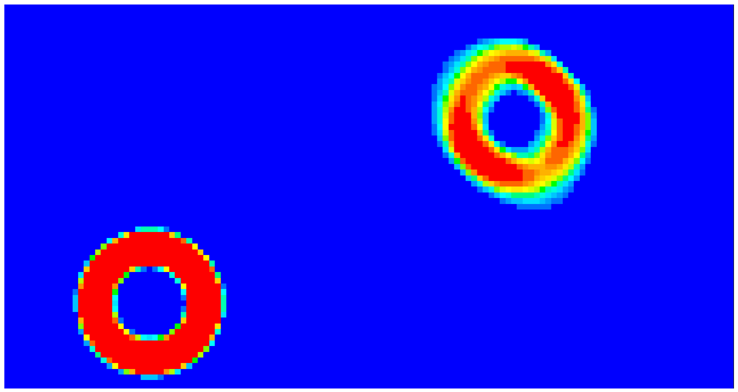
$$\frac{\partial \varepsilon_k}{\partial t} + u_j \frac{\partial \varepsilon_k}{\partial x_i} = S_{\varepsilon k}$$

- 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.

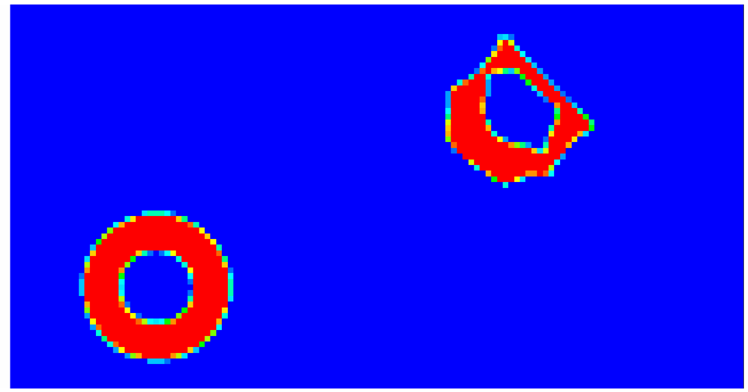
# Interface tracking schemes



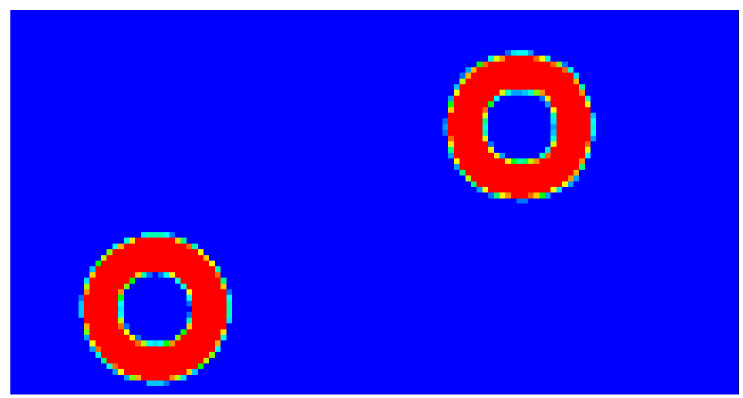
# Comparing different interface tracking schemes



2nd order upwind. Interface is not tracked explicitly. Only a volume fraction is calculated for each cell.



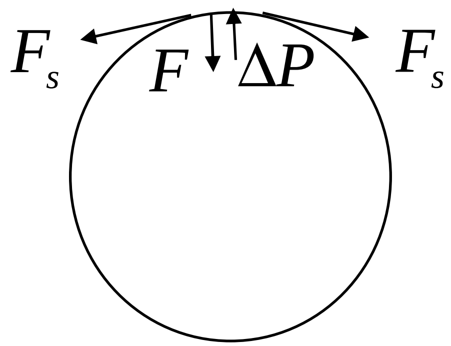
Donor - Acceptor



Geometric reconstruction

# Surface tension

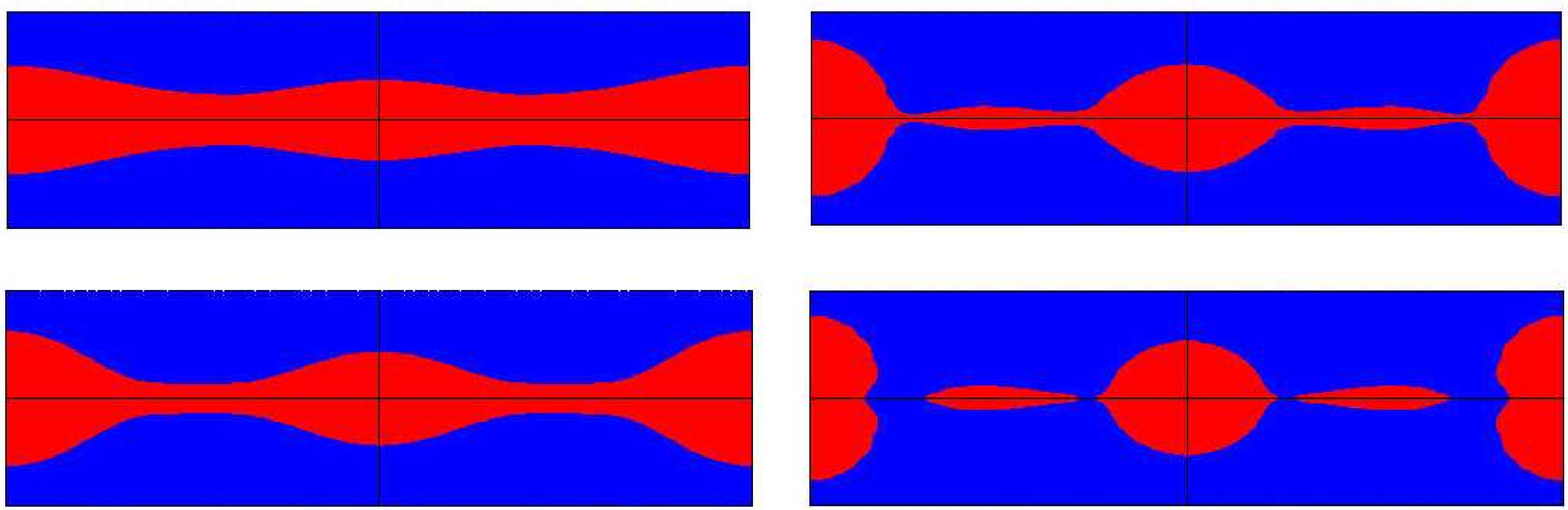
- Surface tension along an interface arises from attractive forces between molecules in a fluid (cohesion).
- Near the interface, the net force is radially inward. Surface contracts and pressure increases on the concave side.
- At equilibrium, the opposing pressure gradient and cohesive forces balance 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.

$$\mathbf{Re} = \frac{\rho U L}{\mu}$$

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

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

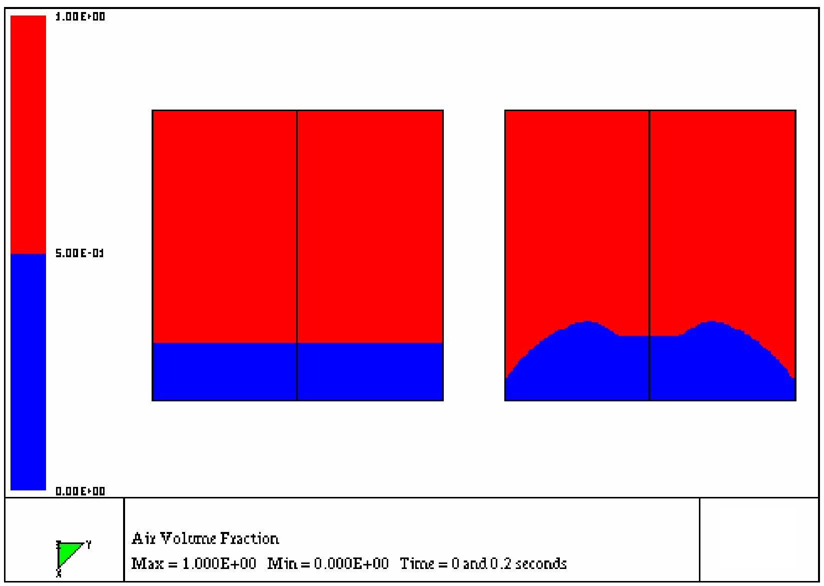
- For Re >> 1, evaluate the Weber number.

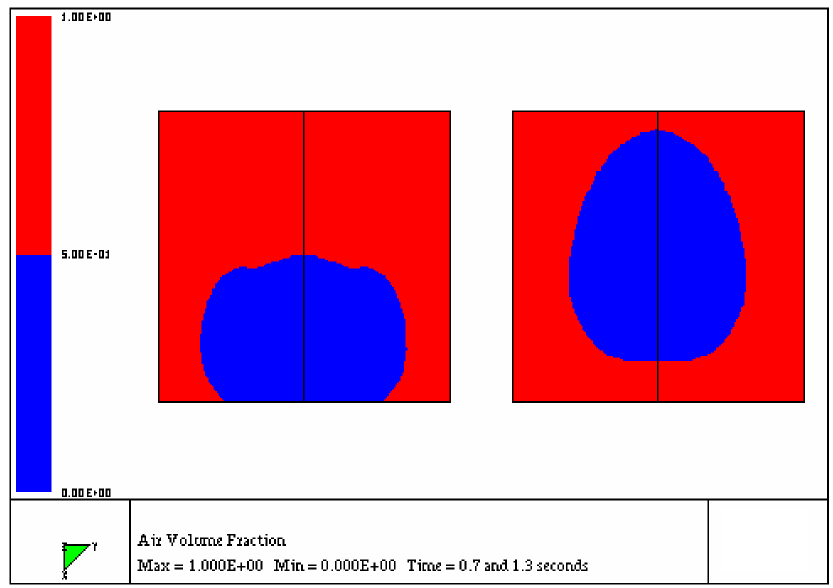
$$\mathbf{We} = \frac{\sigma}{\rho L U^2}$$

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

# Wall adhesion

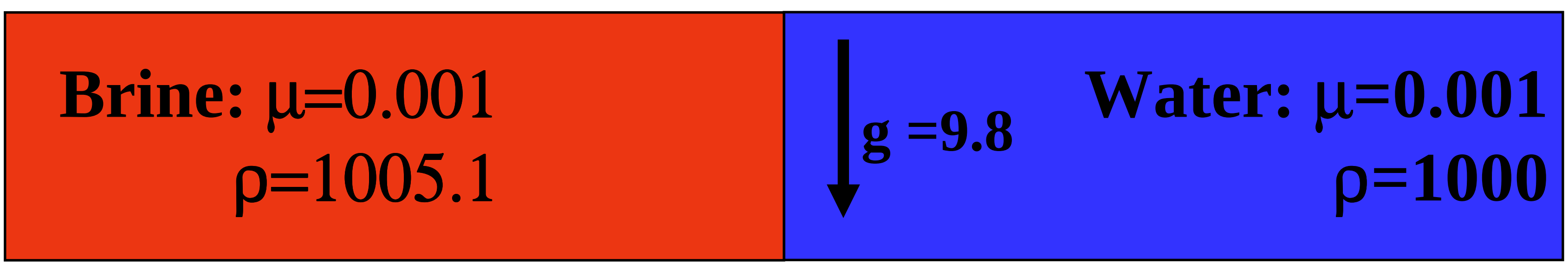
- Large contact angle (> 90°) is applied to water at bottom of container in zero-gravity field.
- An obtuse angle, as measured in water, will form at walls.
- As water tries to satisfy contact angle condition, it detaches from bottom and moves slowly upward, forming a bubble.



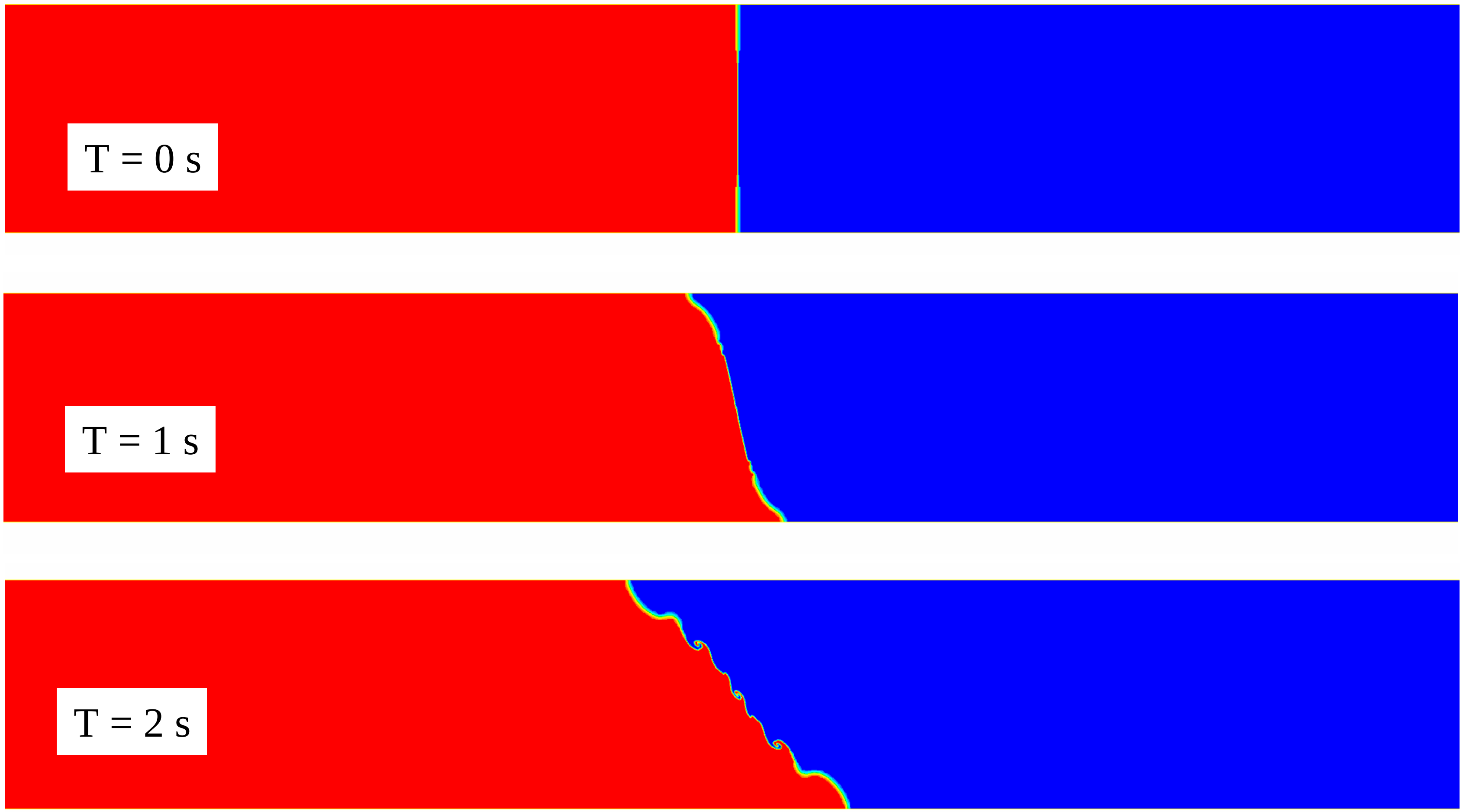



# Modeling of the gravity current

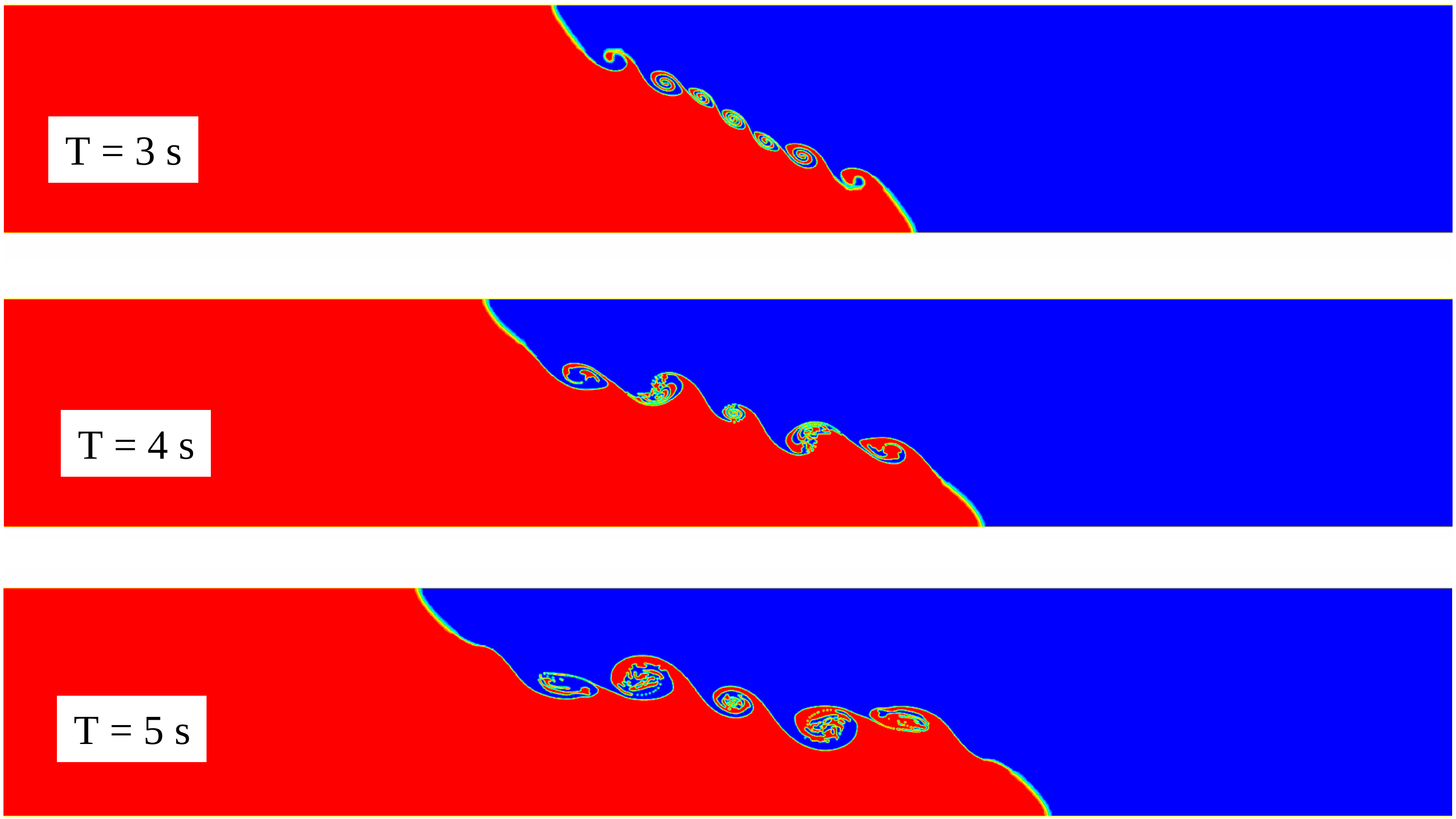
- Mixing of brine and fresh water.
  - 190K cells with hanging nodes.
  - Domain: length 1m, height 0.15m.
  - Time step: 0.002 s.
  - PISO algorithm.
  - Geometric reconstruction scheme.
  - QUICK scheme for momentum.
  - Run time ~8h on an eight-processor (Ultra2300) network.



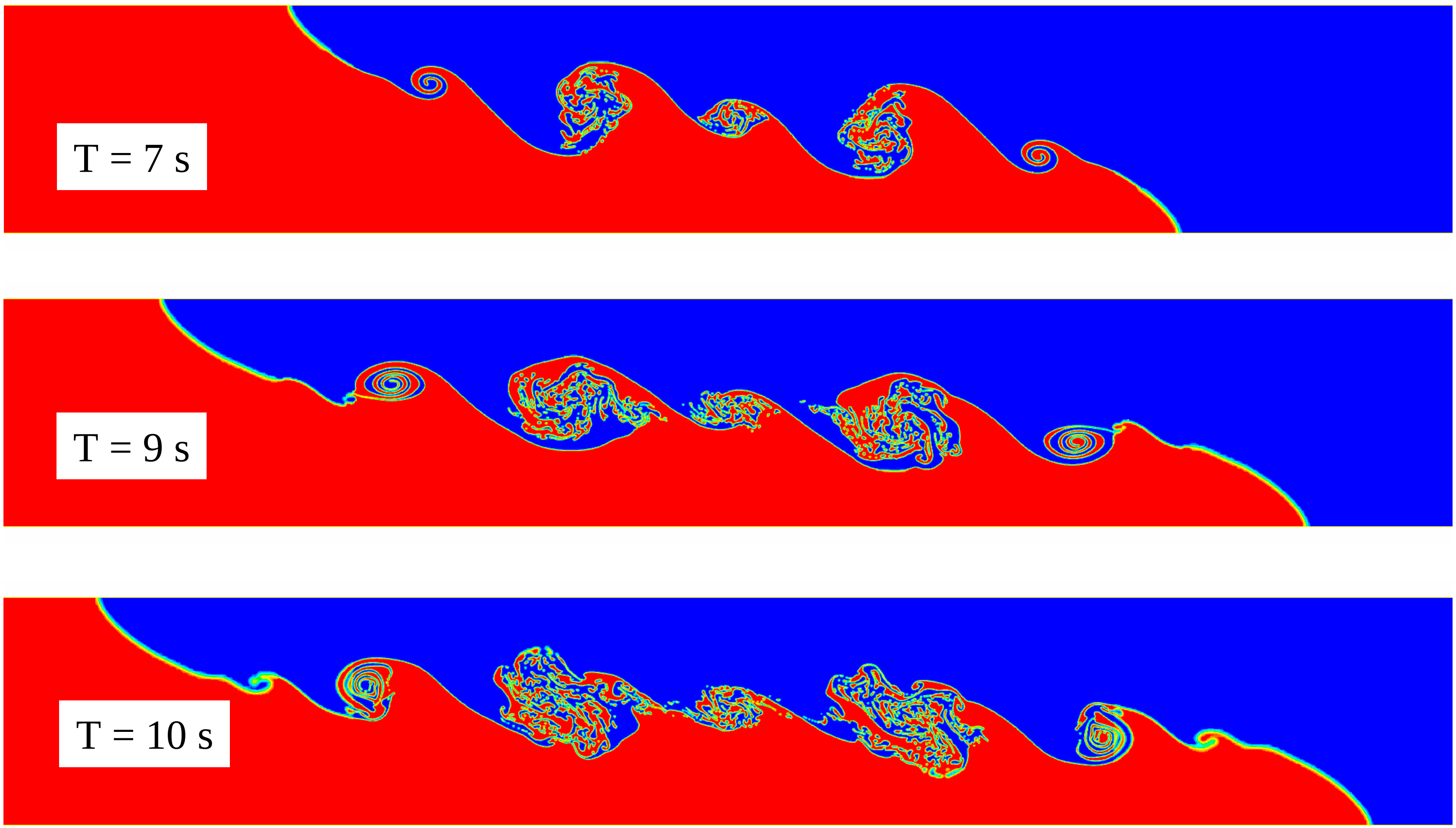
# Gravity current (1)



# Gravity current (2)

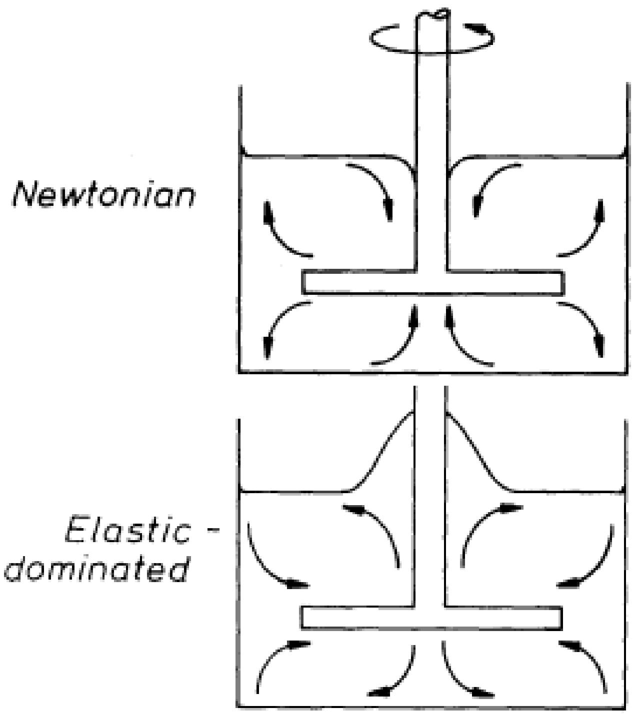


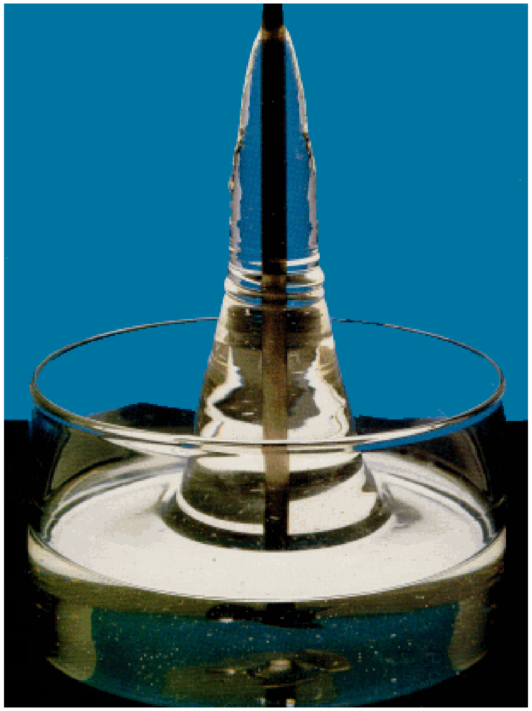
# Gravity current (3)



# 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.



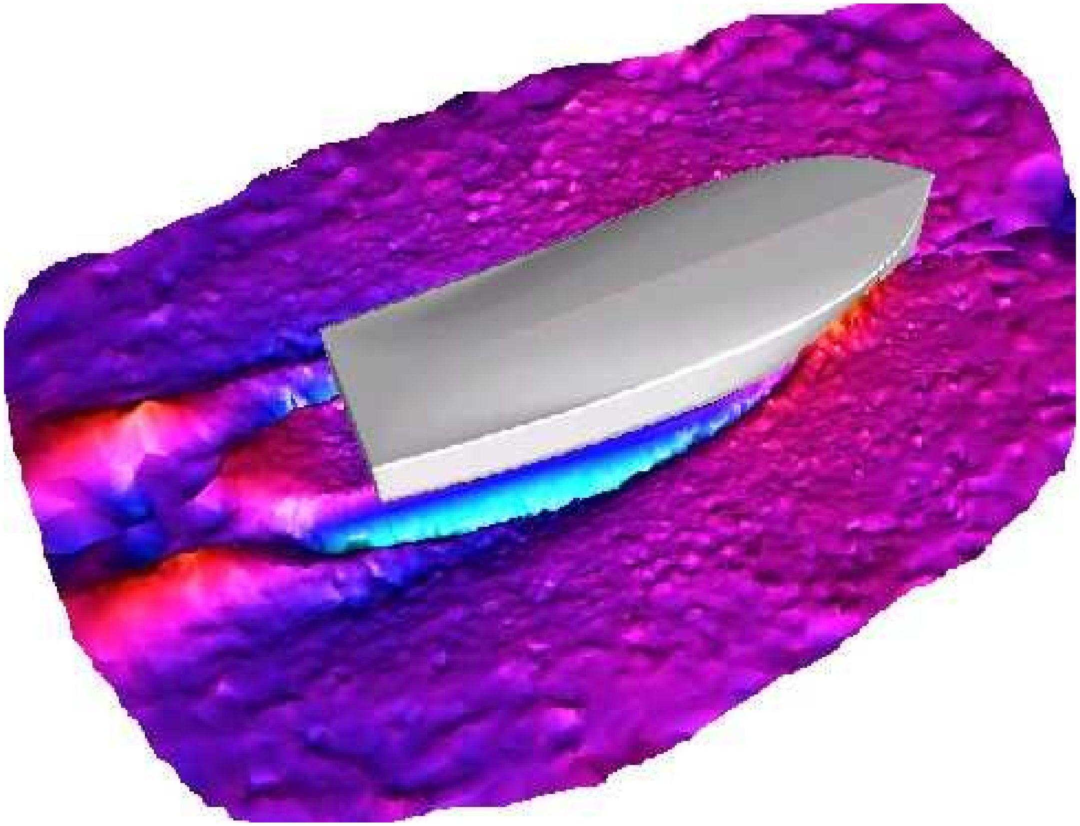



# Visco-elastic fluids - blow molding

- 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:

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

  - $\Delta$t 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.