Volume Of Fluid Model

Advanced Multiphase Modeling Course

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Outline

- Overview
- Inputs and examples
- Solution strategies and common mistakes

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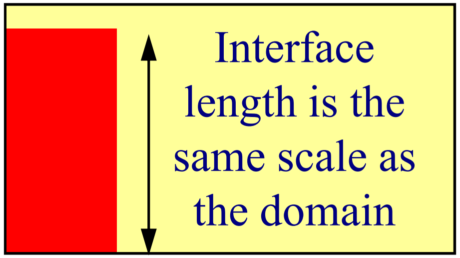
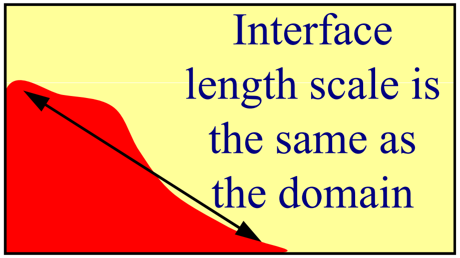
Applicability of the Volume of Fluid Model

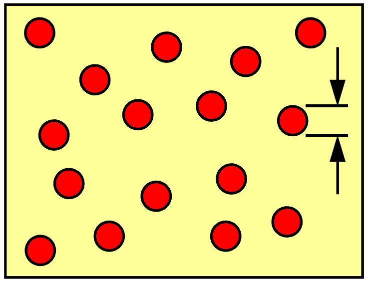
- VOF model is used to model immiscible fluids with clearly defined interface.
  - Two gases cannot be modeled since they mix at the molecular level.
  - Liquid/liquid interfaces can be modeled as long as the two liquids are immiscible.
- VOF is not iate if interface length is small compared to a computational domain
- 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

VOF Applicable





VOF Not Applicable



Interface length is much smaller than domain

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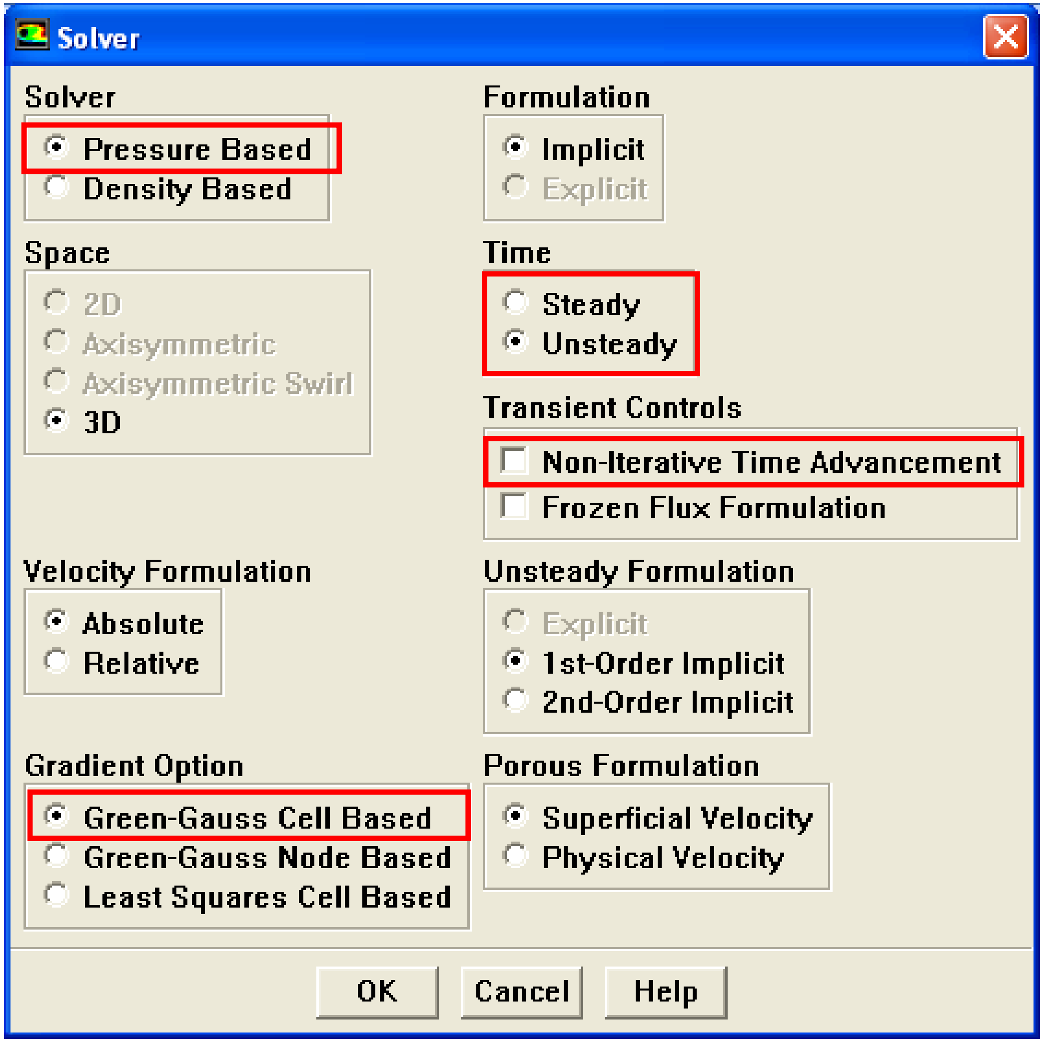
Volume of Fluid Model Inputs

- Solver
  - Only pressure-based solver is available.
  - Green-Gauss Cell Based should only be used with VOF model, other gradient options were not tested with VOF model.
  - VOF model can be run in both Steady and Unsteady mode (unsteady mode is most often used).
  - Non-Iterative Time Advancement (NITA) may be used with VOF model for unsteady mode.



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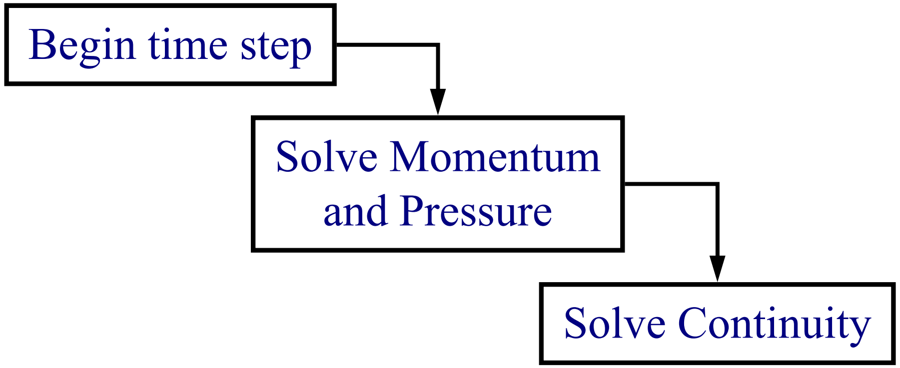
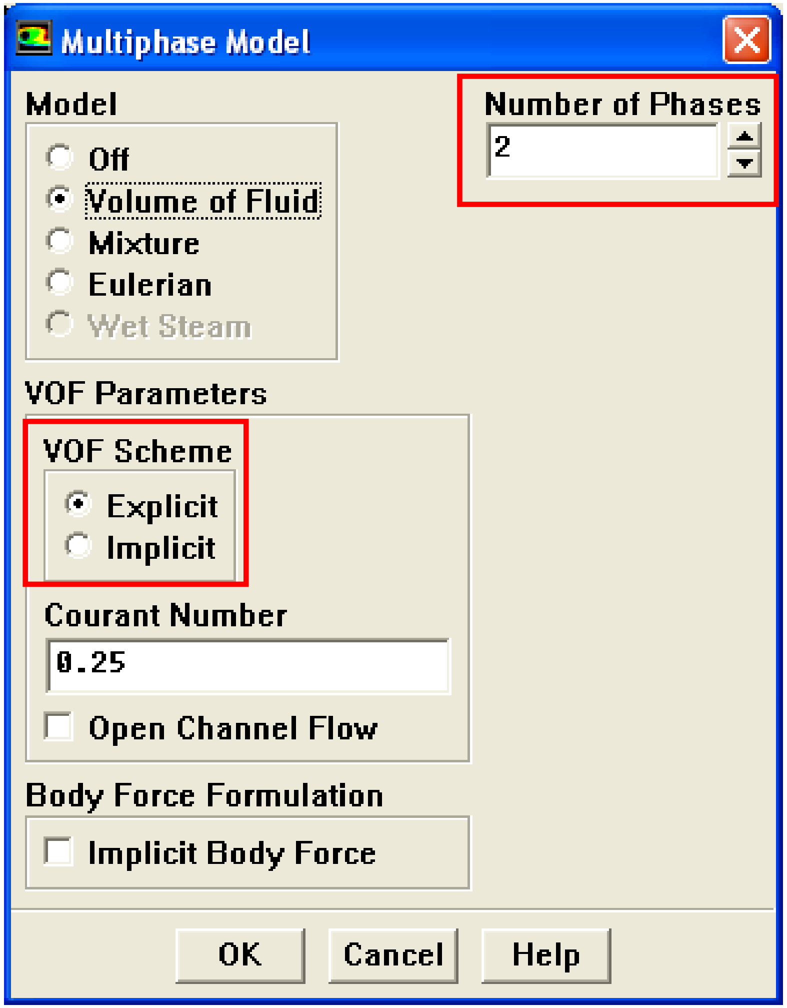
Volume of Fluid Model Inputs

- Multiphase Model
  - Arbitrary number of phases are allowed.
  - VOF Scheme – controls how phase continuity (interface tracking) equation is solved.
  - Explicit VOF – Default and used only with unsteady simulation which is also default





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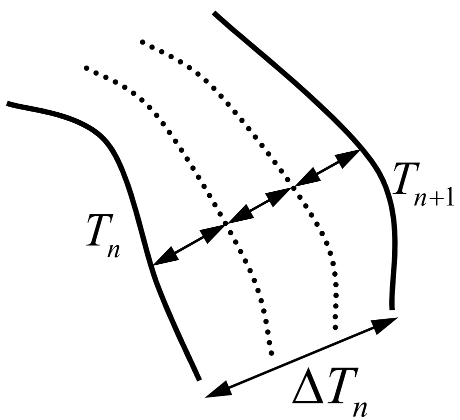
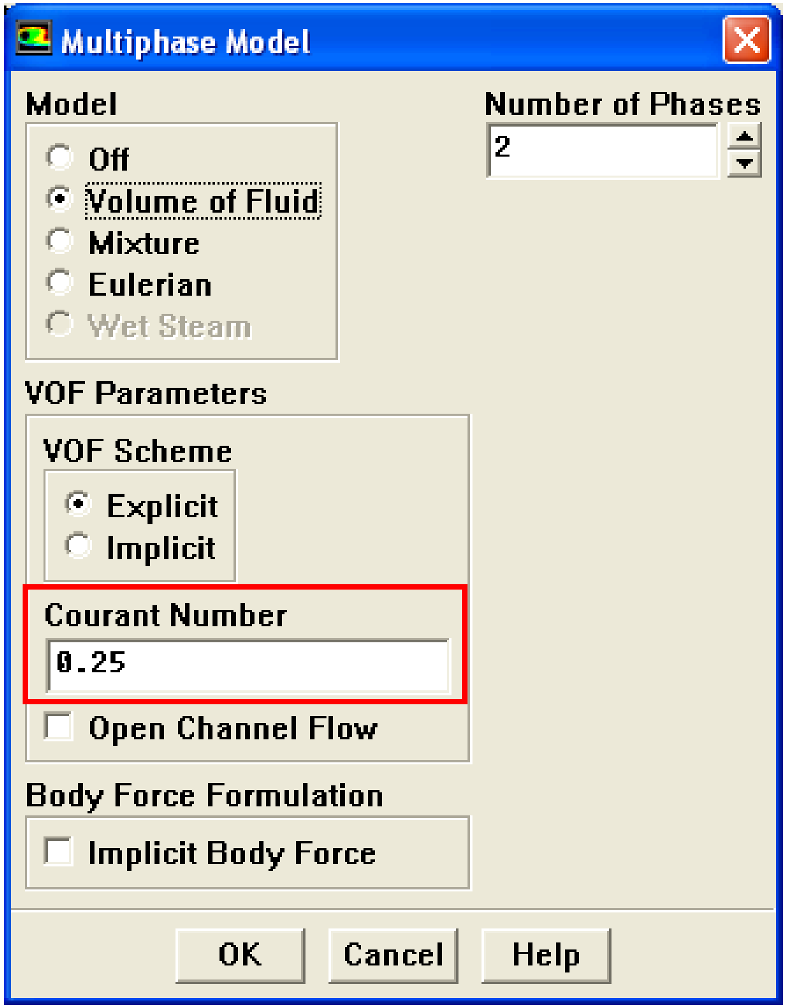
Volume of Fluid Model Inputs

- Multiphase Model (cont'd)
  - Explicit scheme solves the continuity equation in sub time steps.
  - Number of sub time steps is dictated by the value of the Courant number.
  - The default value 0.25 is robust and should not be changed.



Interface location update during one time step



Volume of Fluid Model Inputs

- Multiphase Model (cont'd)
  - Implicit scheme solves phase continuity equation in sub time steps together with momentum and pressure.

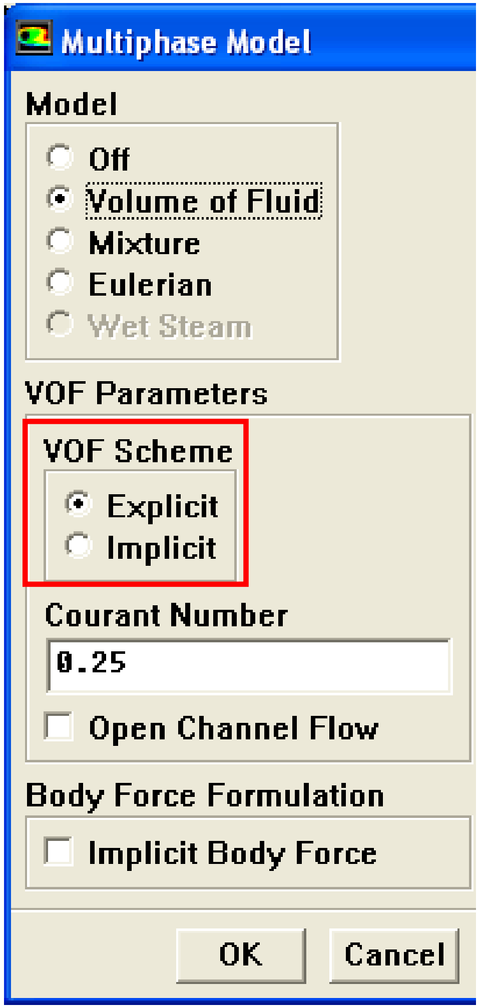
$$\frac{\partial(\rho_q \alpha_q)}{\partial t} + \nabla \cdot (\rho_q \alpha_q \mathbf{v}) = S_{\alpha_q} + \sum_{p=1}^{n} (m_{pq} - m_{qp})$$

Explicit time discretization

$$\frac{(\rho_q \alpha_q)^{n+1} - (\rho_q \alpha_q)^{n}}{\partial t} + \sum_{nb} \nabla \cdot (\rho_q \alpha_q \mathbf{v})^{n} = \left[S_{\alpha_q} + \sum_{p=1}^{n} (m_{pq} - m_{qp}) \right]^{n}$$

Implicit time discretization

$$\frac{(\rho_q \alpha_q)^{n+1} - (\rho_q \alpha_q)^{n}}{\partial t} + \sum_{nb} \nabla \cdot (\rho_q \alpha_q \mathbf{v})^{n+1} = \left[S_{\alpha_q} + \sum_{p=1}^{n} (m_{pq} - m_{qp}) \right]^{n}$$



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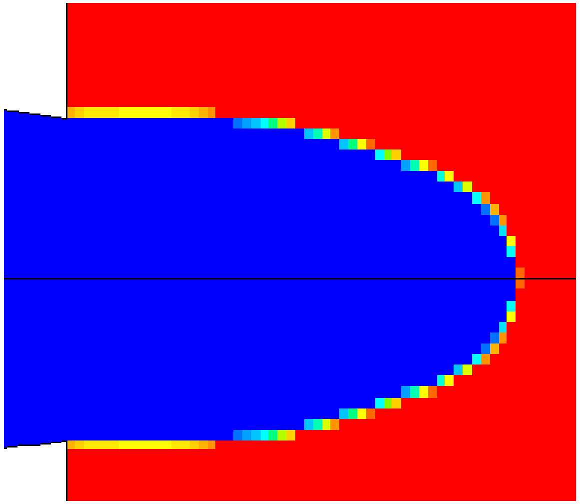
Volume of Fluid Model Inputs

- Tradeoff between implicit and explicit VOF schemes
  - Advantages of explicit scheme
    - Allows use of Geo-Reconstruct discretization scheme for VOF. This scheme renders a clear, crisp interface without numerical diffusion.
    - Should be used in simulation of flows where surface tension is important because of highly accurate curvature calculation.
  - Disadvantages of explicit scheme
    - Poor convergence for skewed meshes.
    - Poor convergence if phases are compressible.



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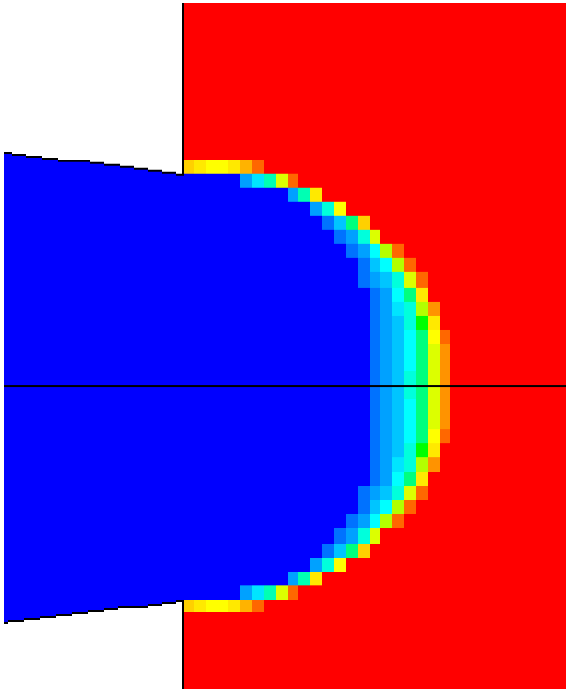
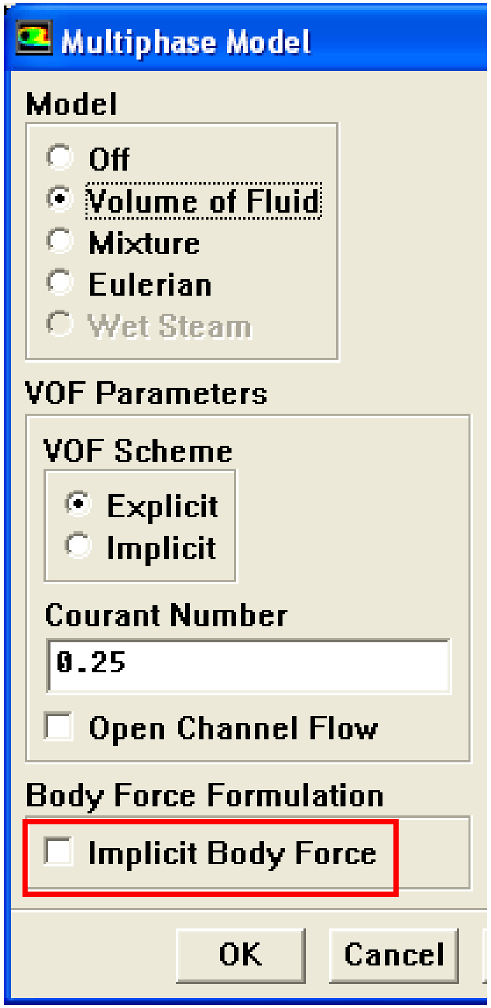
Volume of Fluid Model Inputs

- Tradeoff between implicit and explicit VOF schemes
  - Advantages of implicit scheme
    - Does not have Courant number limitation – can be run with large time steps or in steady state mode.
    - Can be used with poor mesh quality and for complex flows (e.g. compressible).
  - Disadvantages of implicit scheme
    - Numerical diffusion of interface does not allow accurate prediction of interface curvature so accurate prediction of flows where surface tension is important is not feasible.



Volume of Fluid Model Inputs

- Implicit body force
  - Designed for flows with large body forces such as gravity acting on phases with large density difference or strong rotational acceleration
  - The force is handled in robust numerical manner



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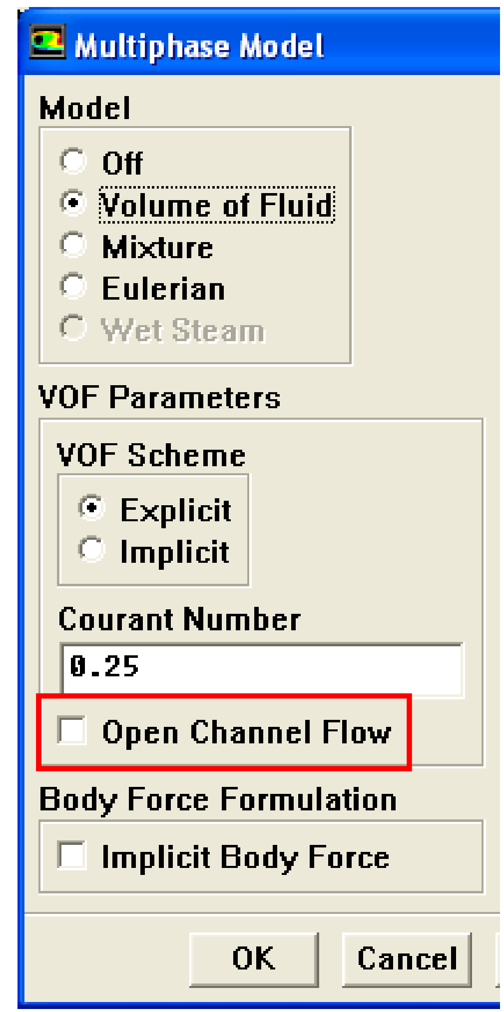
Volume of Fluid Model Inputs

- Open Channel Flow option
- Applicable to flows where both inertia and gravity are dominant with known depths of the liquid at the inlets or outlets
  - Example – Ship moving through the sea at depth y_{in} and speed V_{in}
  - Prescribe y_{in} and V_{in} at inlet and y_{out} at the outlet.
  - If $Fr = V_{in}\,(g\,y_{in})^{-0.5} > 1$, then choice of y_{out} does not matter – flow supercritical, if $Fr < 1$, then choice of y_{out} influence solution (subcritical flow).
- One can specify either y_{in} and V_{in} (convection driven) or height difference (gravity driven) between y_{in} and y_{out}.



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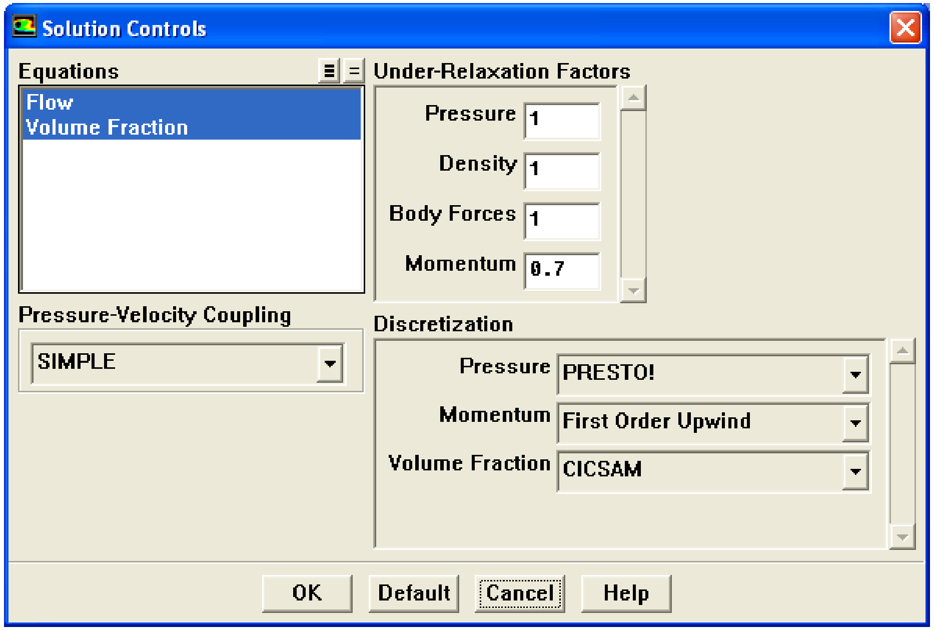
Volume of Fluid Model Inputs

- Material properties
  - If viscosity ratio of phases is of order 10^5 or higher, convergence problem may arise
  - Typical scenario – Mold filling problem of non-Newtonian polymer with high viscosity at lower temperatures
  - Solution
    - Increase smaller viscosity so the ratio is below 10^5 as either constant or through UDF
    - Use Explicit multiphase scheme with special volume fraction discretization scheme – CICSAM



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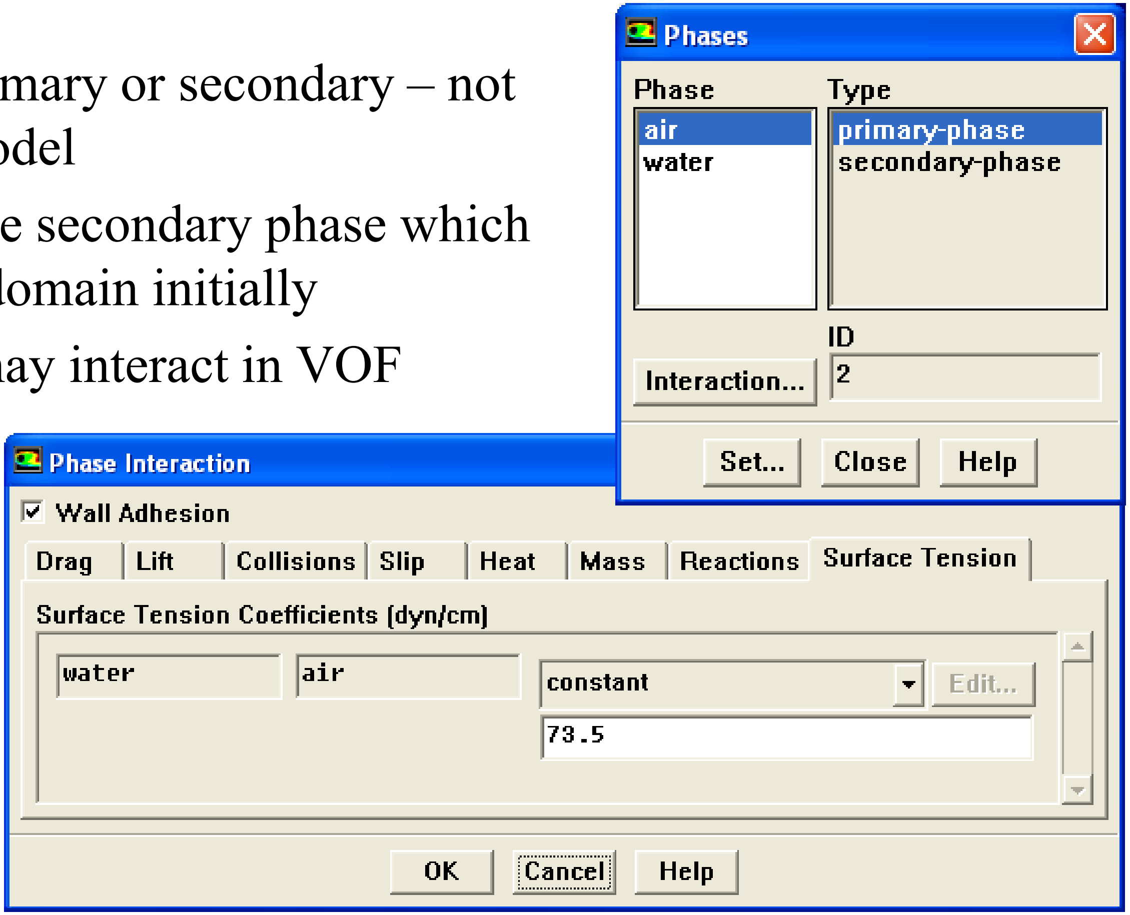
Volume of Fluid Model Inputs

- Phases
  - Any phase can be primary or secondary – not important in VOF model
  - Usual practice to have secondary phase which has less presence in domain initially
  - Three ways phases may interact in VOF
    - Mass exchange
    - Heterogeneous reactions
    - Surface tension with wall adhesion effect



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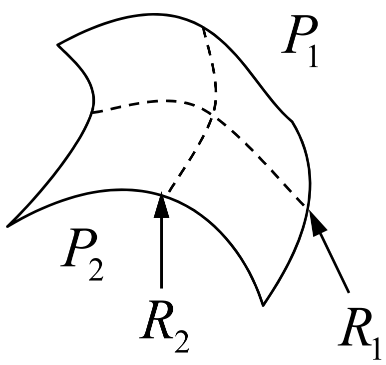
Volume of Fluid Model Inputs

- Phases (cont'd)
  - Mass exchange is described in tutorial
  - Surface tension coefficient can be constant or function of variables (often temperature)
  - Surface tension along an interface arises from attractive forces between molecules in a fluid (cohesion)
  - Pressure difference is equal to surface tension coefficient times sum of inverse curvature radii



For 3D: $$P_2 - P_1 = \sigma\left(\frac{1}{R_1} + \frac{1}{R_2}\right)$$

For 2D: $$P_2 - P_1 = \frac{2\sigma}{R}$$

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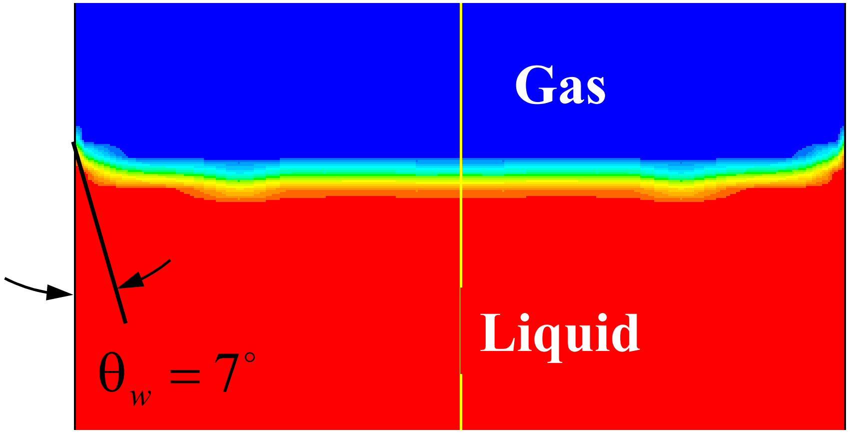
Volume of Fluid Model Inputs

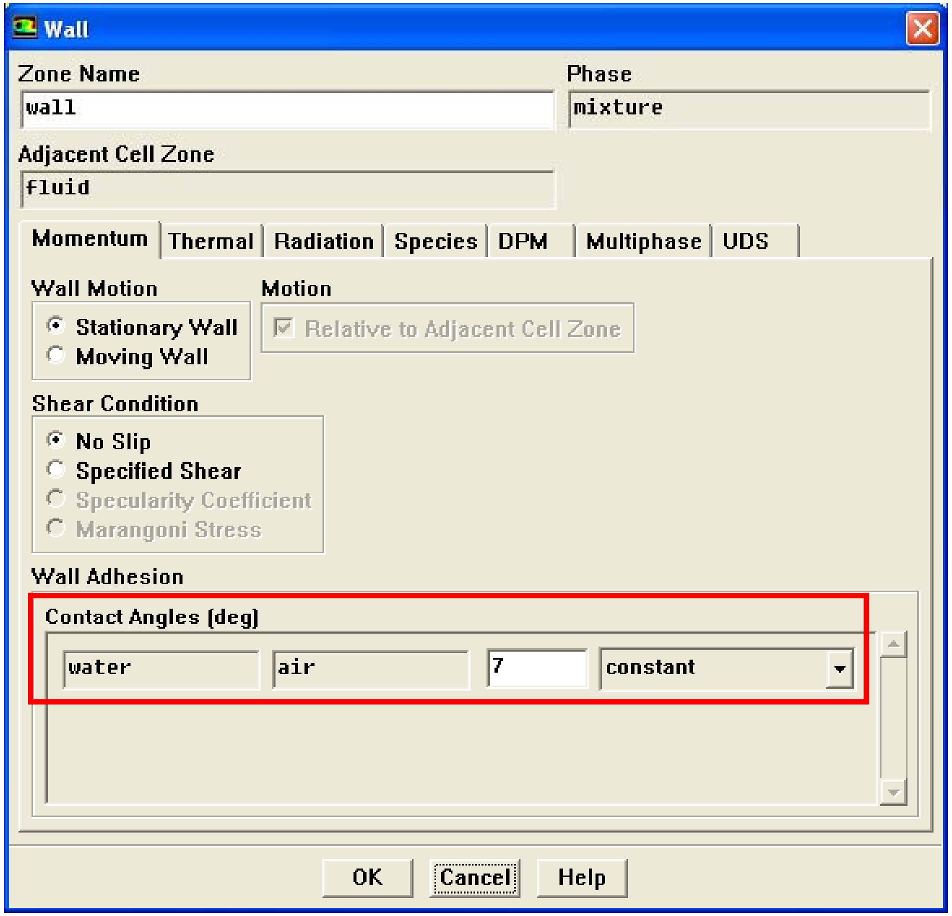
- Phases (cont'd)
  - To determine significance of surface tension, first evaluate the Reynolds number: $$\mathrm{Re} = \frac{\rho U L}{\mu}$$
  - For Re << 1, evaluate the Capillary number: $\mathrm{Ca} = \dfrac{\mu U}{\sigma}$
  - For Re >> 1, evaluate the Weber number: $\mathrm{We} = \dfrac{\sigma}{\rho L U^2}$
    - Surface tension is important when We >>1 or Ca<< 1.
  - Surface tension is modeled using an additional source term in the momentum equation

$$\vec{F}_{pq} = \frac{\sigma\left(\alpha_p \rho_p \kappa_p \nabla \alpha_p\right) + \left(\alpha_q \rho_q \kappa_q \nabla \alpha_q\right)}{\frac{1}{2}\left(\rho_p + \rho_q\right)}, \quad \kappa = \nabla \cdot \left(\frac{\nabla \alpha}{\left\|\nabla \alpha\right\|}\right)$$

Volume of Fluid Model Inputs

- Phases (cont'd)
  - Wall adhesion force is a measure of the cohesive forces existing between fluid and bounding wall
  - Important for prediction of meniscus shapes





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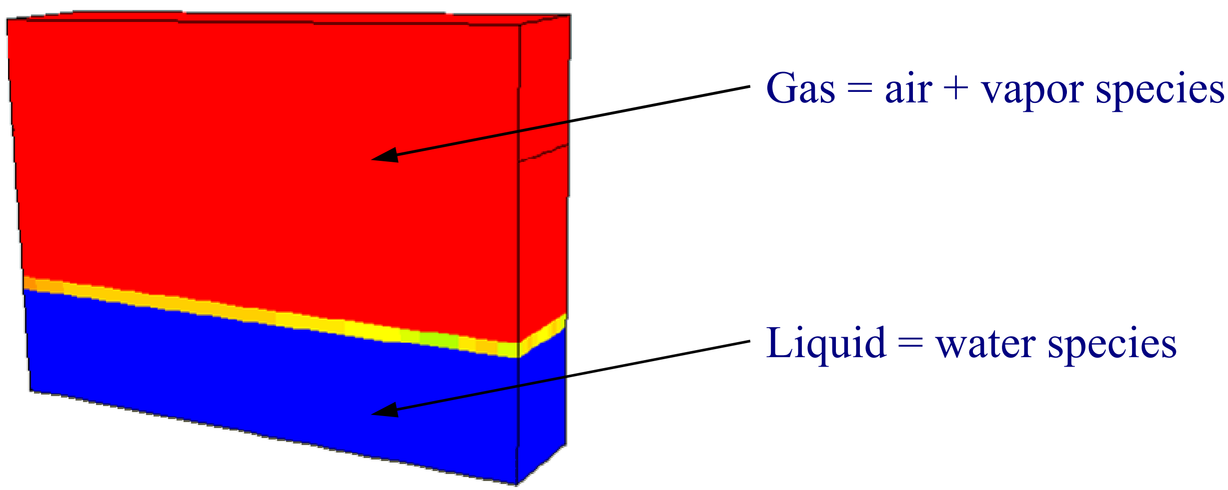
Volume of Fluid Model Inputs

- Phases (cont'd)
  - Heterogeneous reactions
    - Example of heterogeneous reaction simulating evaporation of water into vapor-air atmosphere
    - Gas phase is mixture of vapor and air species
    - Liquid phase is mixture of water



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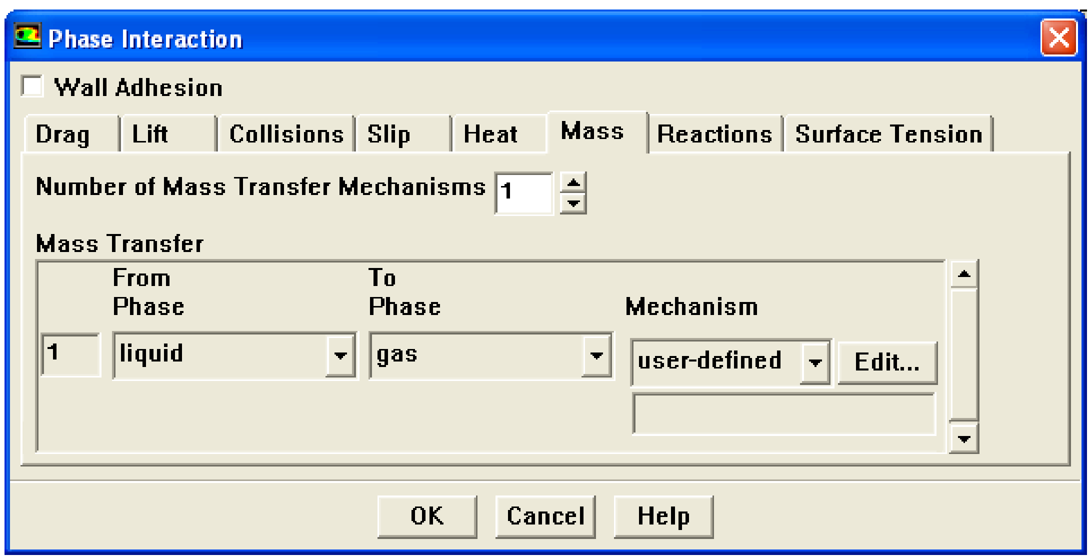
Volume of Fluid Model Inputs

- Phases (cont'd)
  - Heterogeneous reactions
    - Evaporation reaction is represented as heterogeneous reaction
    - Evaporation rate is calculated via UDF from ideal gas theory

$$\dot{m} = k \cdot \left\|\nabla\alpha\right\| \left(P_{\mathrm{sat}} - P_{\mathrm{part,vap}}\right) \quad \left[\frac{\mathrm{kg}}{\mathrm{m}^3 \cdot \mathrm{sec}}\right]$$



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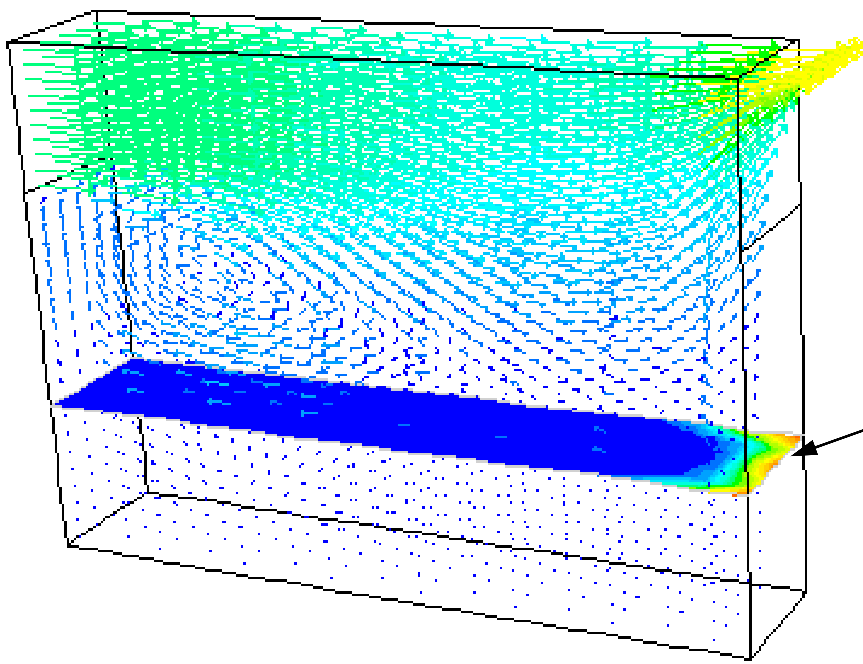
Volume of Fluid Model Inputs

- Phases (cont'd)
  - Vector along with free surface and evaporation rate at free surface



Evaporation rate at free surface

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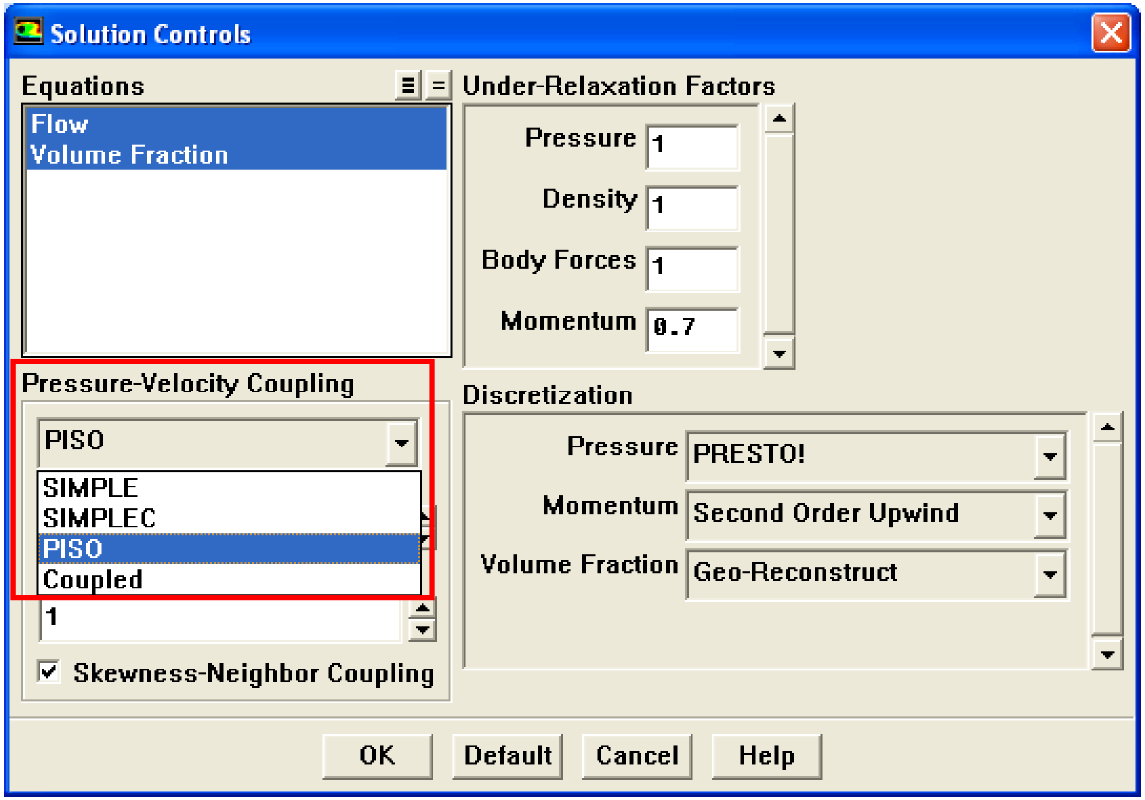
Volume of Fluid Model Inputs

- Numerical settings for explicit formulation
- Pressure-velocity coupling
  - PISO recommended for non-complicated flows
  - SIMPLE or SIMPLEC for compressible flows or flows in closed domains



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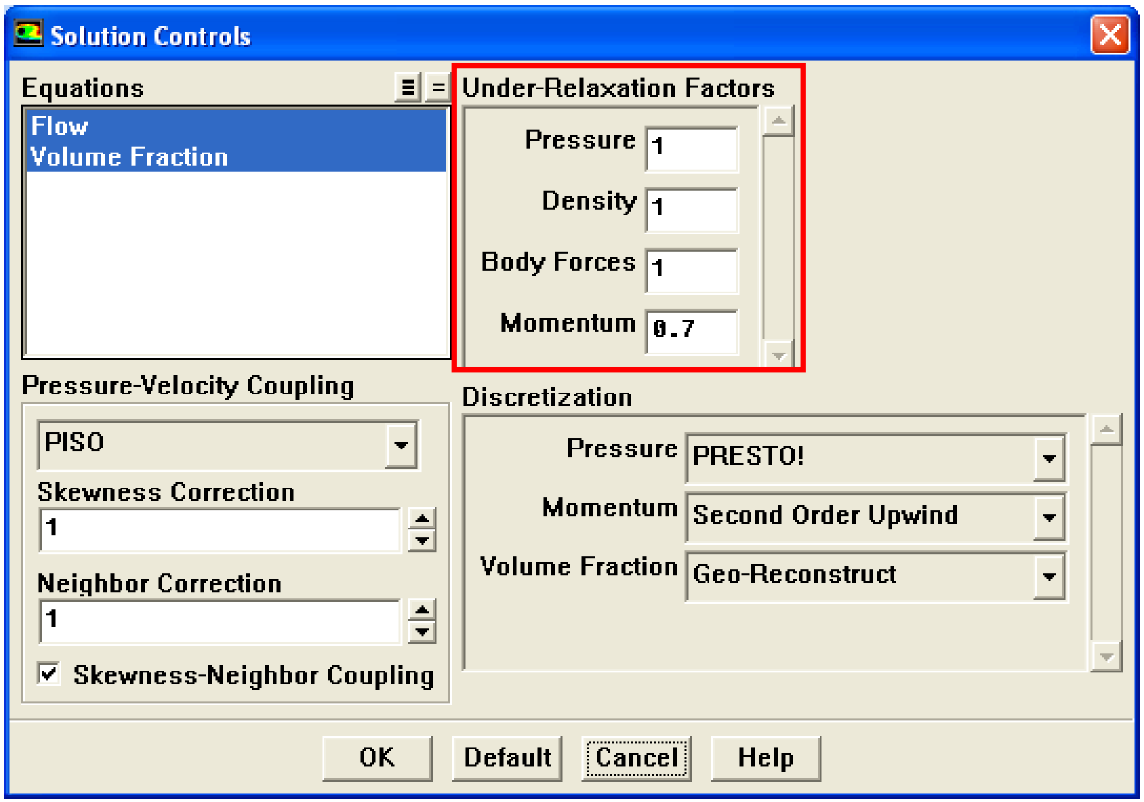
Volume of Fluid Model Inputs

- Numerical settings for explicit formulation (cont'd)
- URFs
  - Conservative settings are shown.
  - For simple cases, pressure and momentum URFs can be increased
  - NOTE – No URF for VOF as it is solved explicitly with substeps



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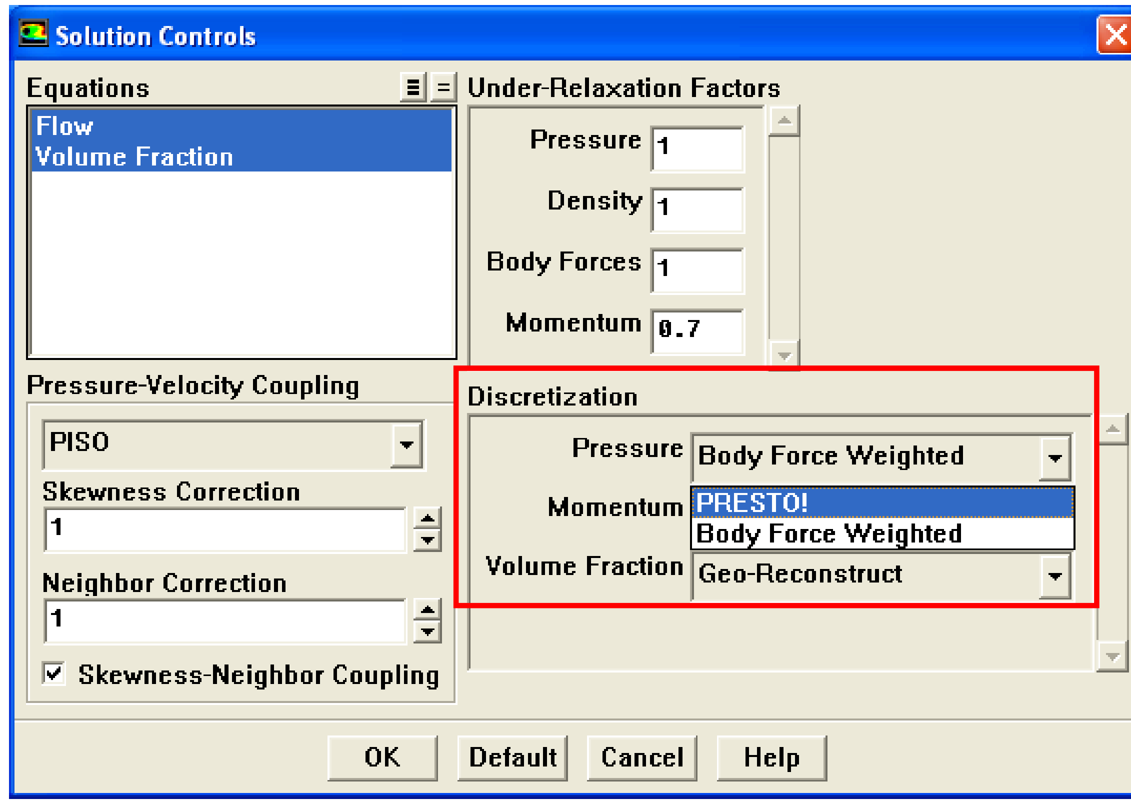
Volume of Fluid Model Inputs

- Pressure discretization
  - Body Force Weighted for high body force (rotation)
  - PRESTO! is recommended otherwise



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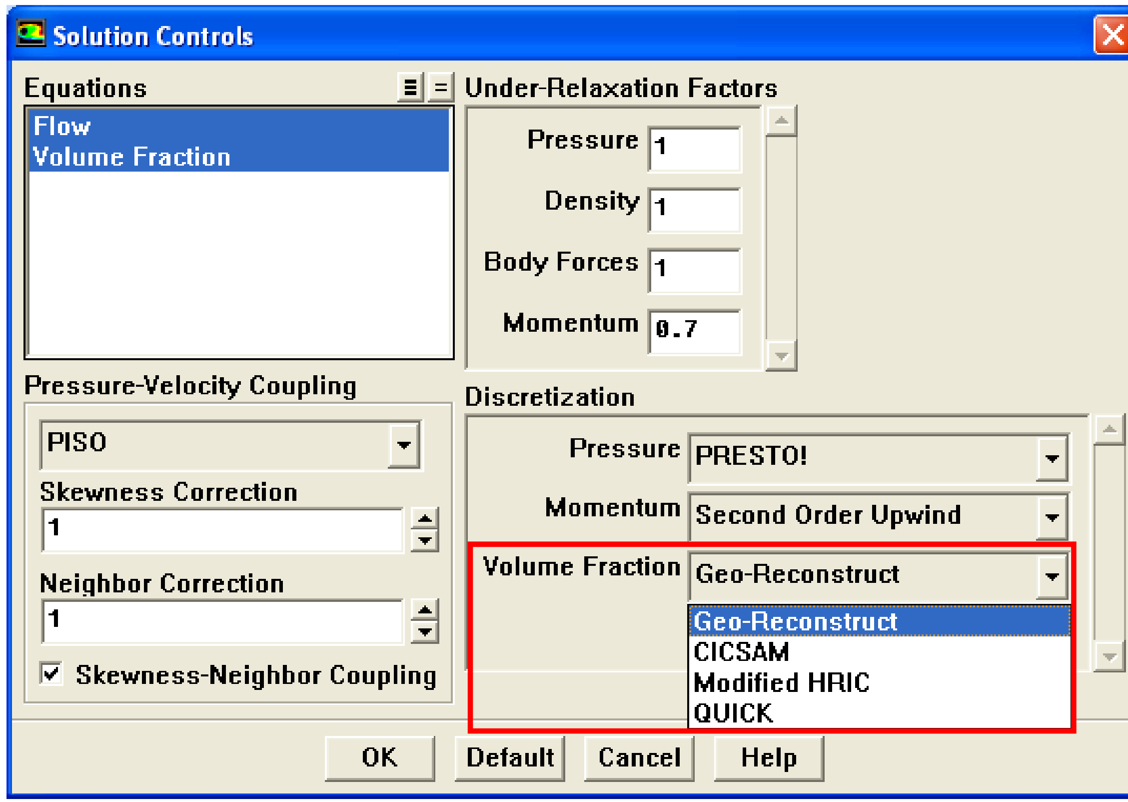
Volume of Fluid Model Inputs

- Numerical settings for explicit formulation (cont'd)
- VOF discretization
  - **Geo-Reconstruct** – Default, no numerical diffusion, high accuracy curvature, needs high quality grid.
  - **CICSAM** – Should be used for large jobs, high efficiency for parallel computations.
  - **HRIC** – recommended when schemes above fail.



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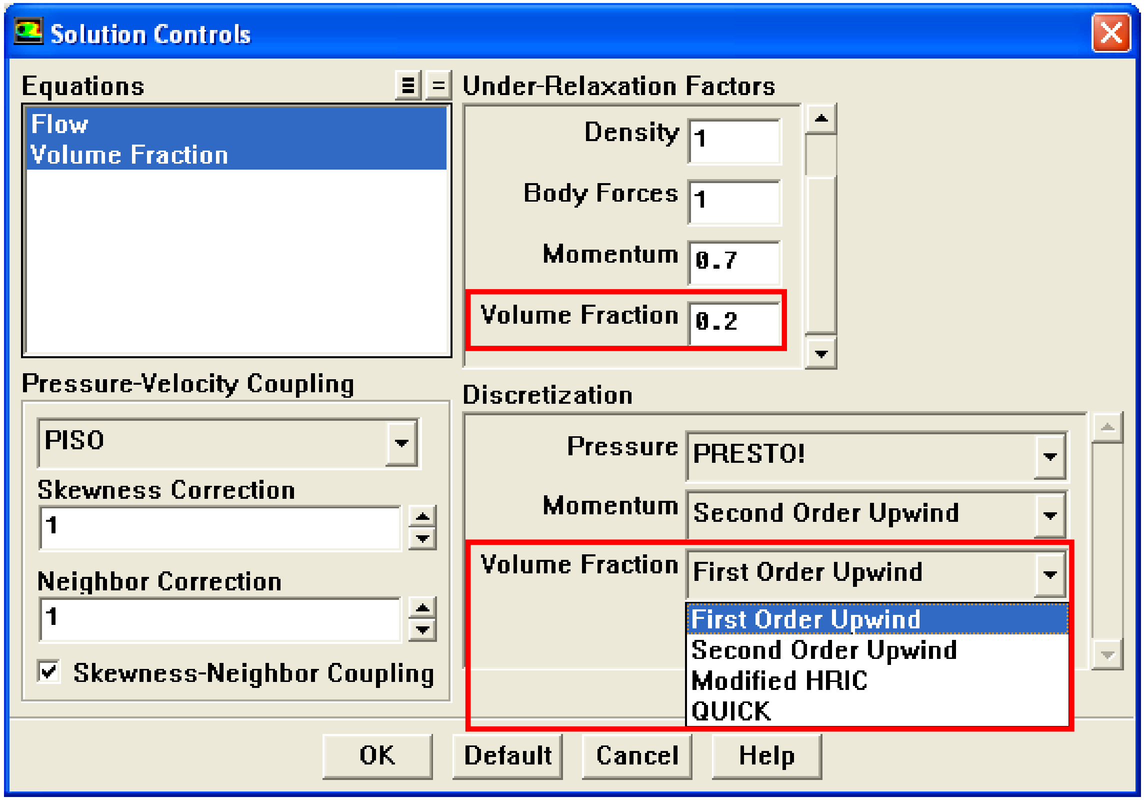
Volume of Fluid Model Inputs

- Numerical settings for implicit formulation
- URF for VOF equation is added – can be increased from default value
- HRIC is recommended discretization scheme for VOF



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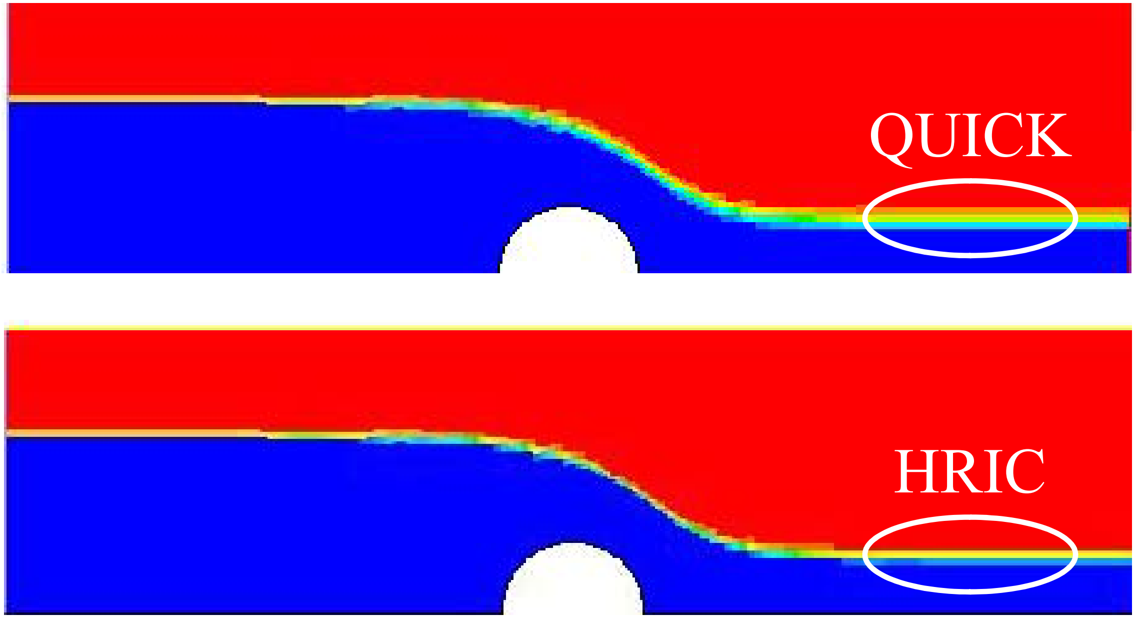
Volume of Fluid Model Inputs

- Numerical settings for implicit formulation
- Example of lower numerical diffusion by HRIC scheme in comparison to QUICK scheme for VOF discretization



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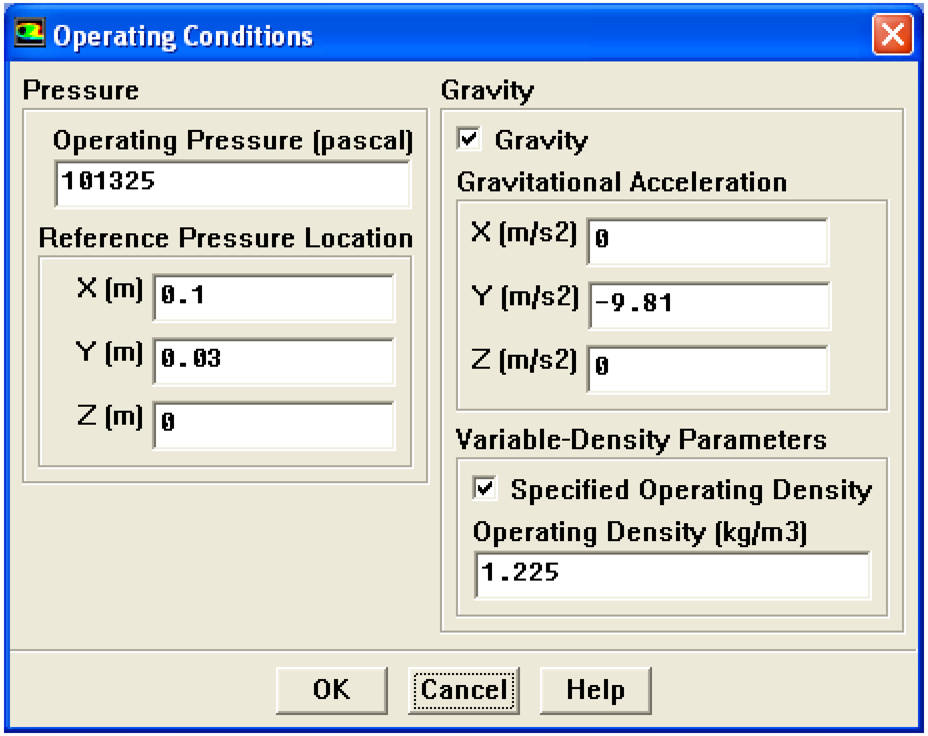
Volume of Fluid Model Inputs

- Operating conditions
  - Reference Pressure Location should not be changed.
  - Specified Operating Density – lowest density of the phases.
  - If phases are compressible – lowest density at operating pressure



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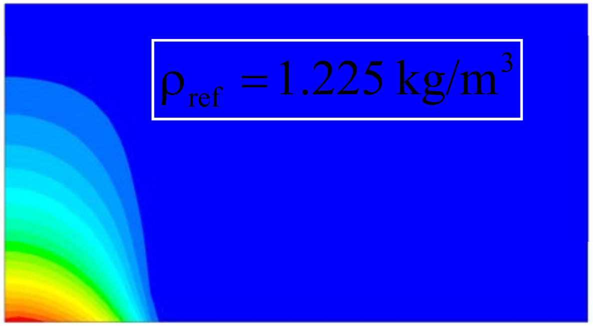
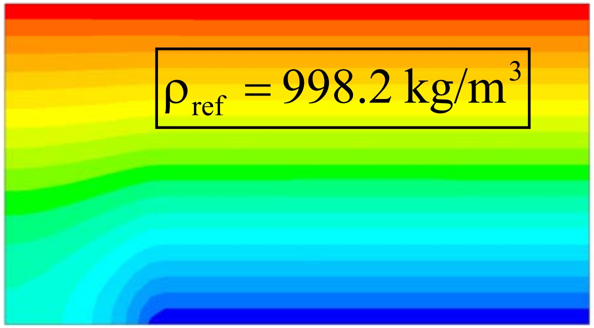
Volume of Fluid Model Inputs

- Operating conditions (cont'd)
  - Example of dam break
  - Choice of large density as reference will result in incorrect pressure distribution





Pressure distribution in the dam break example

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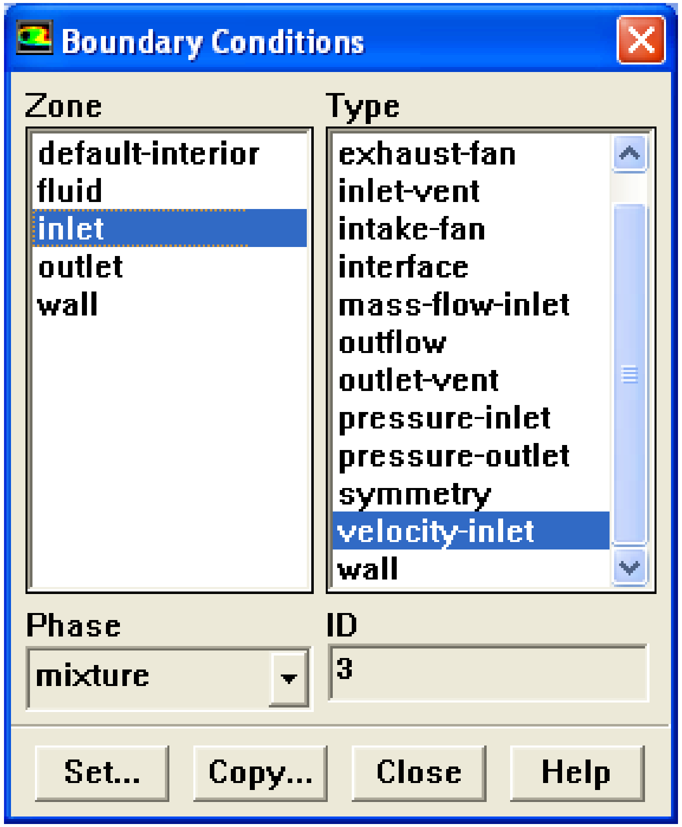
Volume of Fluid Model Inputs

- Boundary conditions - inlets and outlets
  - Allowed inlet boundary conditions:
    - Velocity-inlet – Used for incompressible flows only.
    - Pressure inlet
    - Mass flow inlet
  - Allowed outlet boundary conditions:
    - Pressure outlet
    - Outflow is incorrect for VOF although FLUENT will allow it



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Volume of Fluid Model Inputs

- How to prescribe boundary conditions
  - Velocity inlet – Only one phase can enter; therefore, only one phase can have inlet volume fraction set to 1 and nonzero inlet velocity. All inputs for other phases are irrelevant.
  - Mass flow inlet – Same as above. Only one phase can have nonzero mass flow rate. Inputs for all phases are irrelevant.
  - Pressure inlet – Same as above. Only one phase can have inlet volume fraction of 1. Inputs for all other phases are irrelevant.
    - In order so facilitate convergence for pressure inlet, it is advisable to patch VOF of incoming to 1 for the cell layer adjacent to the pressure inlet.

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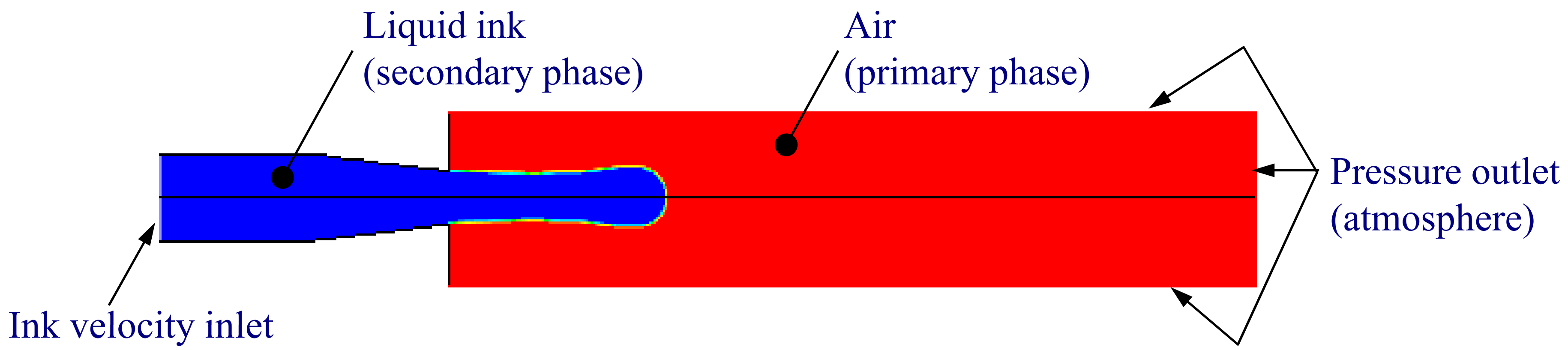
Volume of Fluid Model Inputs

- How to prescribe boundary conditions
  - Pressure outlet
    - Be careful which VOF you specify as backflow VOF!
    - Consider ink jet injected into atmosphere



Backflow VOF of ink phase at atmosphere is zero

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Solution Strategies – Time Dependence

- How to choose transient time step for VOF calculations
  - Time step in Solve panel can be estimated as

$$\Delta t = \frac{V_{\text{cell, min}}^{1/3}}{U}$$

  - Where $V_{\text{cell, min}}$ is obtained from the Grid Check panel and U is the velocity scale of the problem (e.g. inlet velocity).
  - If divergence occurs at first time step, decrease time step by factor of 10 and see if it converges. Ideally, you should converge in about 10-15 iterations.
  - If divergence persists, try switching off Skewness-Neighbor Coupling in the Solution Controls panel.

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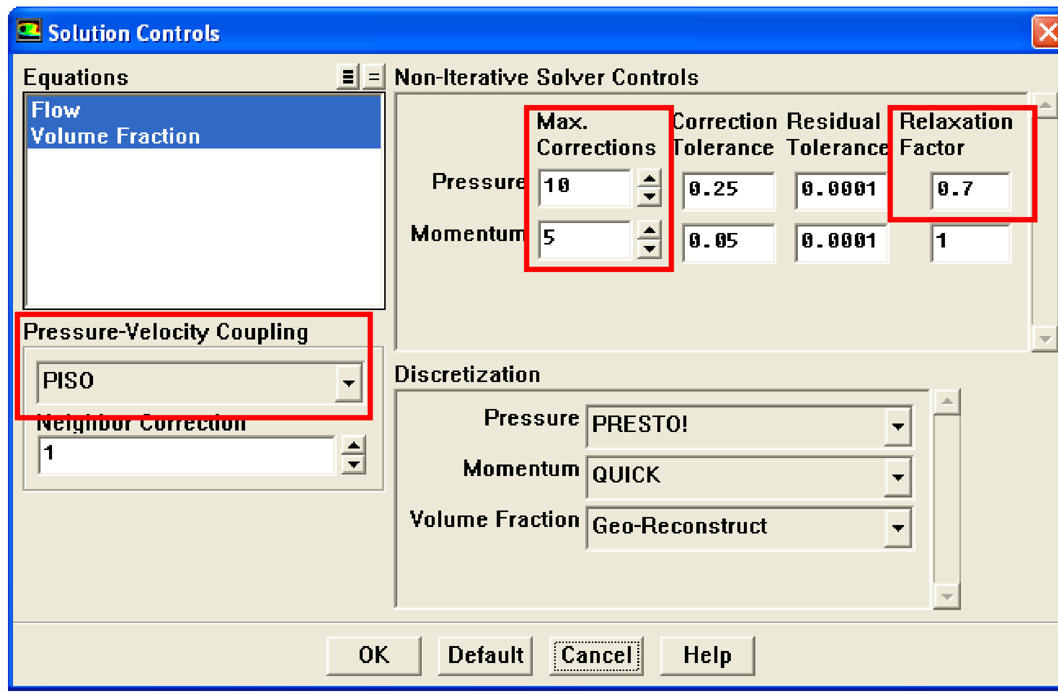
Solution Strategies – Time Dependence

Define → Models → Solver...

- Non-iterative time advancement (NITA) reduces computational effort per time step in comparison with iterative schemes (SIMPLE, PISO)
- Can be used with the VOF model; however, convergence problems may occur. Use variable time steps and reduce Max. corrections number for Momentum and reduce Relaxation Factor for pressure.



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Solution Strategies – Discretization

- Recommended discretization schemes
  - Pressure
    - PRESTO! was specifically developed to handle flows with large density variations and body forces – this is the exact situation with most VOF problems, so PRESTO! should be used in most cases.
    - Body Force Weighted can also be used.
  - Velocity
    - Either First Order Upwind or Second Order Upwind is recommended.

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Solution Strategies – Common Mistakes

- Outflow boundary condition does not exist in multiphase flows.
- At any inlet or outlet, only one phase must enter or exit. This means that on any flow boundary, the volume fraction must be either 0 or 1. No intermediate values should be used.
- Interface update scheme is most sensitive to grid quality. It is advisable to put highest quality mesh in areas where the interface is expected.

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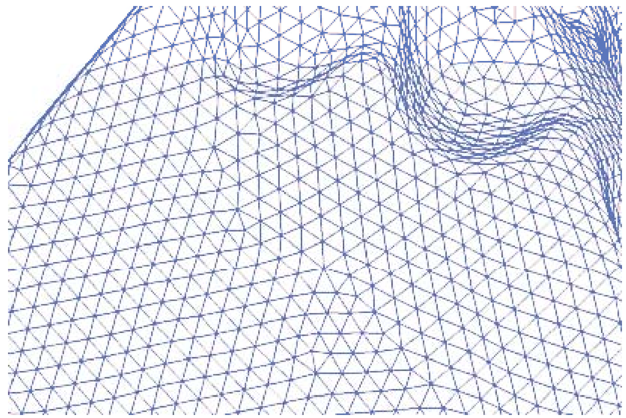
Solution Strategies – Common Mistakes

- Smooth, good quality mesh is essential to good convergence of VOF model.



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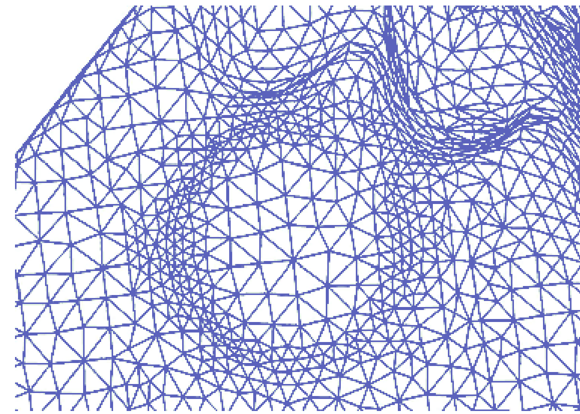
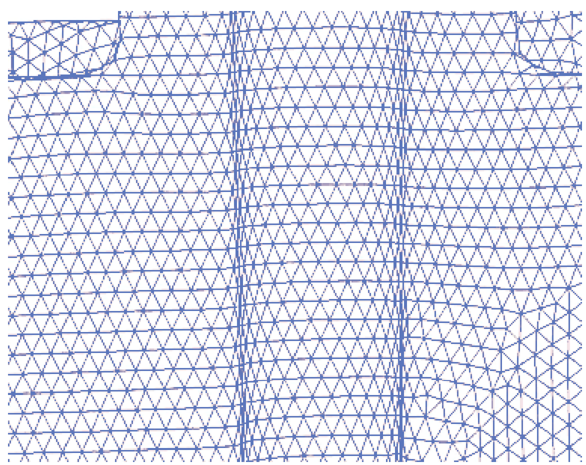


Bad

- Cells which have large skewness, high aspect ratio, or large size variation are detrimental to convergence rate.



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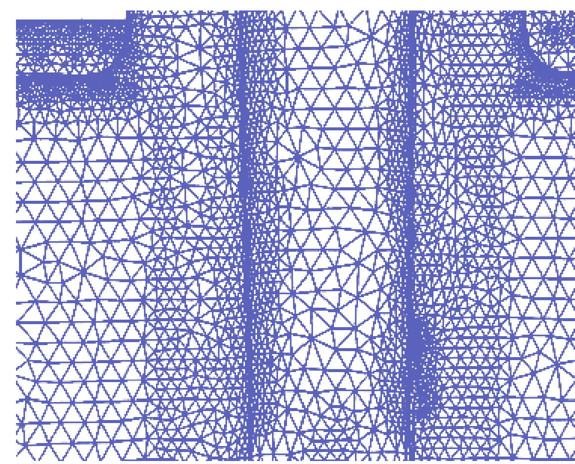

Bad

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VOF Model Examples

Tank Filling
Slug Flow in a Pipe
3D Falling Box
Spinning Gear

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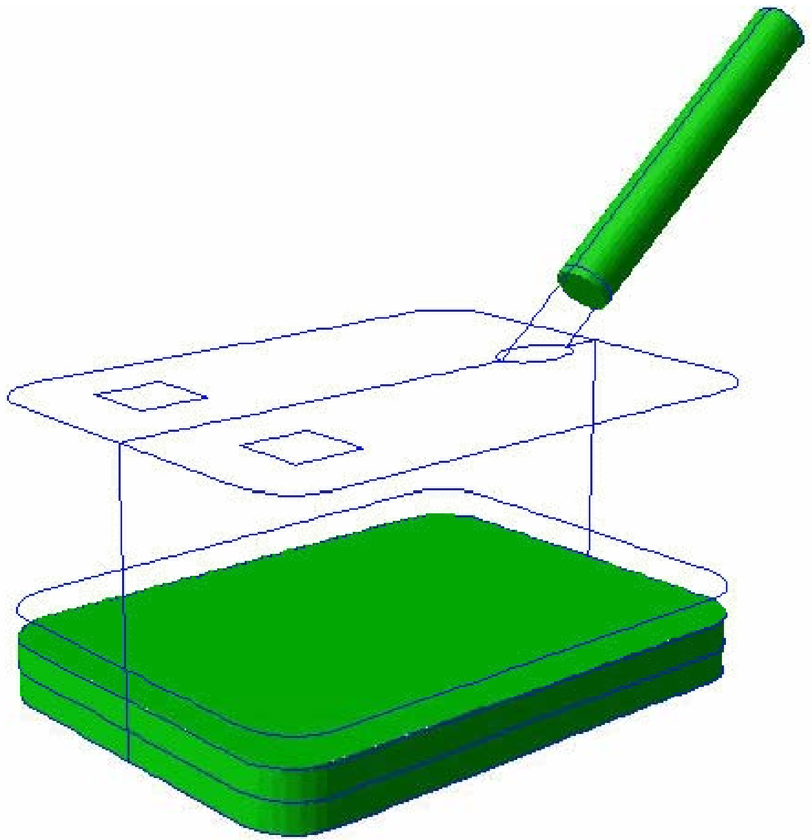
VOF Example – Tank Filling

- Simple filling of a vessel



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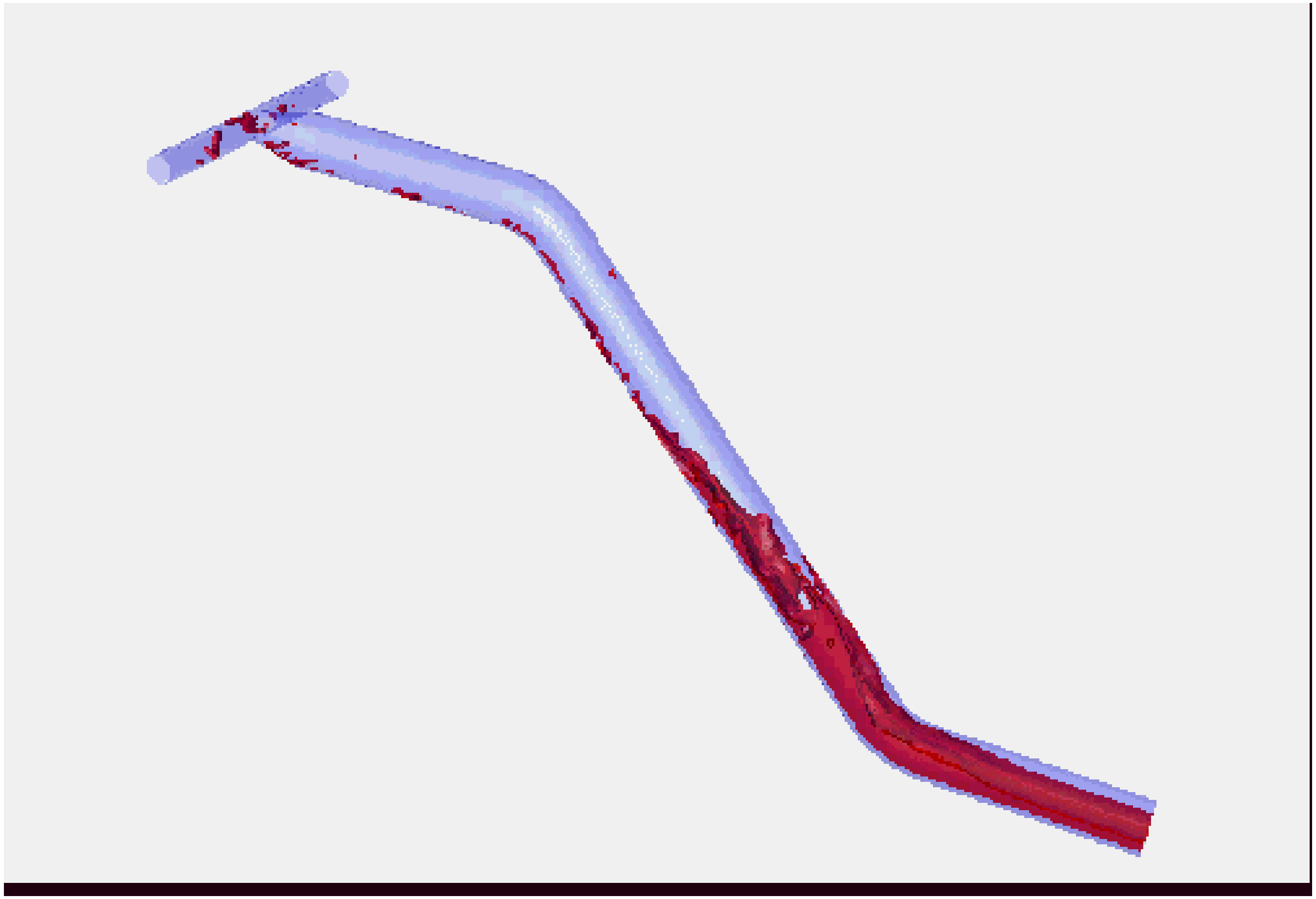
VOF Example – Slug Flow in a Pipe



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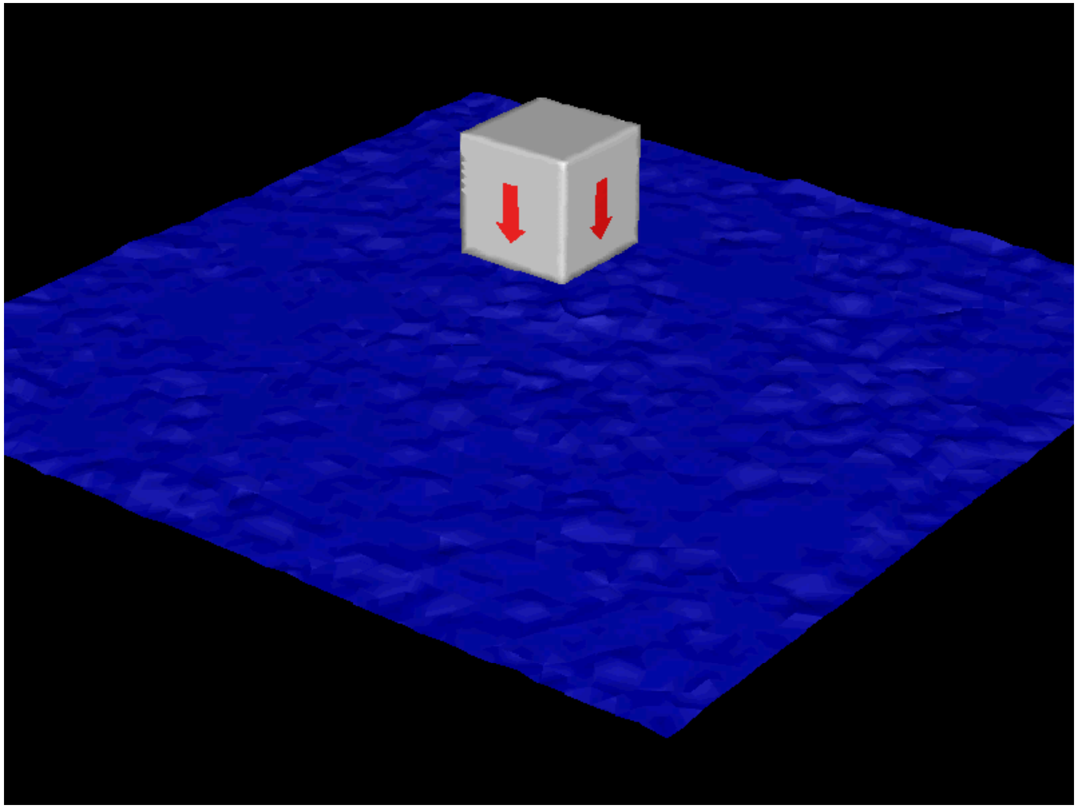
VOF Example – 3D Falling Box

- Deforming mesh capability with VOF model was used to simulate a box falling into liquid.



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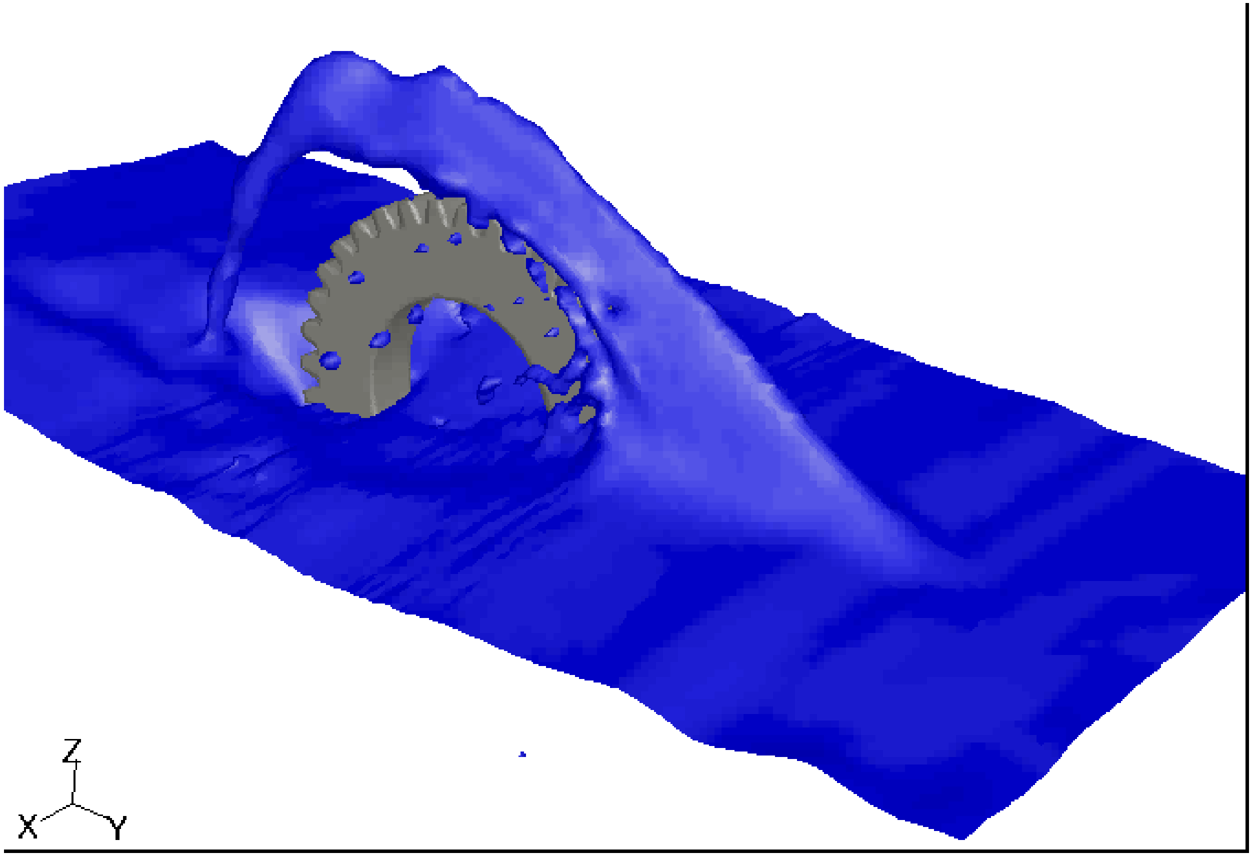
Free Surface Flow around a Spinning Gear

- Sliding mesh model with multiphase VOF



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Summary

- VOF is an Eulerian fixed-grid technique.
- VOF is numerically robust and accurate.
- Available in conjunction with most other FLUENT models.
  - Not available with the following reacting flow models:
    - Eddy dissipation concept
    - Premixed, non-premixed, partially premixed
    - Composition PDF
    - NOx and soot

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