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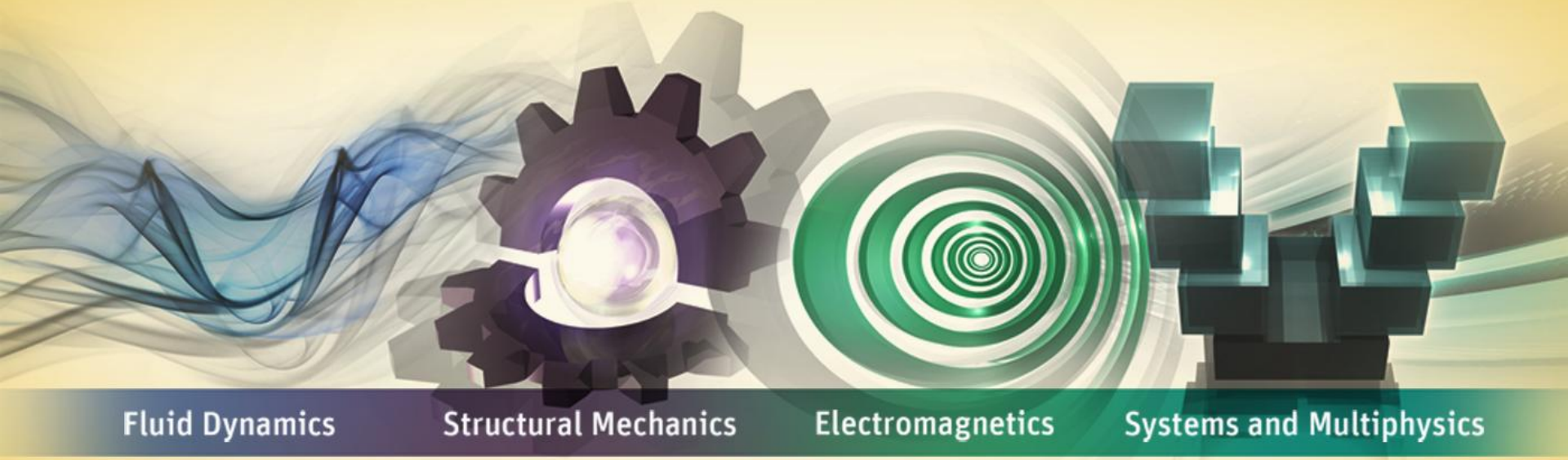
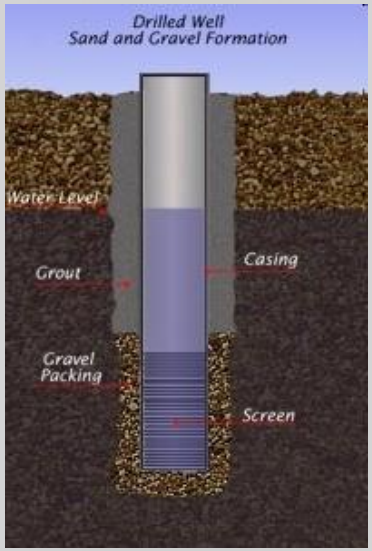
A Solution for Every Multiphase Challenge

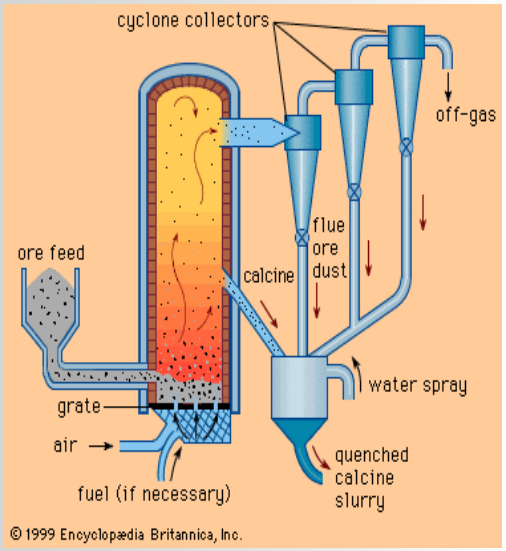


Clinton Smith, PhD
CAE Support and Training
PADT
April 26, 2012

Introduction

- **Multiphase flows are encountered in many industries**
  - Oil and Gas
  - Petroleum refining and Hydrocarbon processing
  - Automotive and Aviation
  - Metallurgy, Mining and Pharmaceutical





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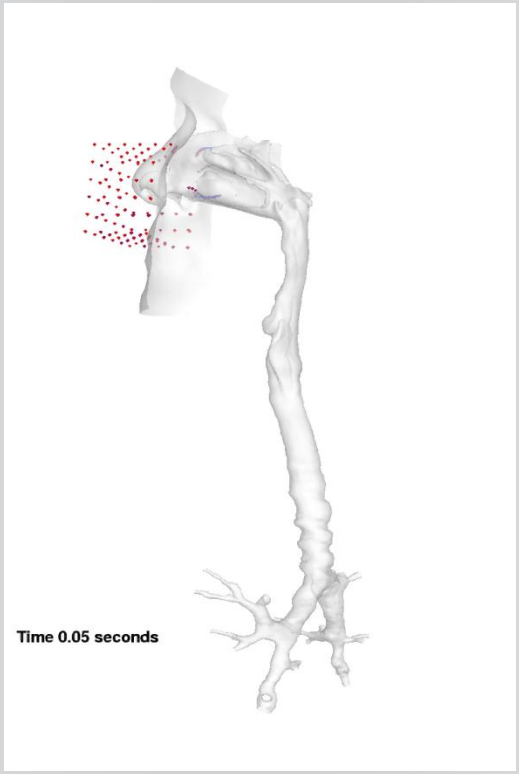
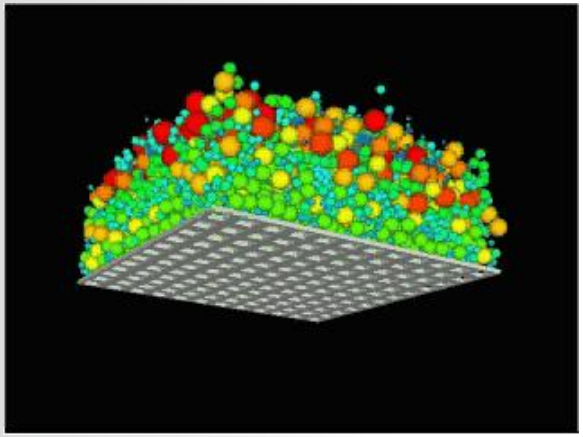
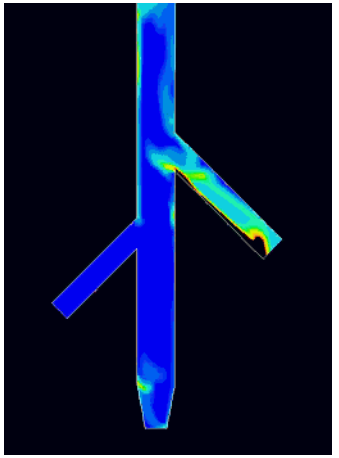
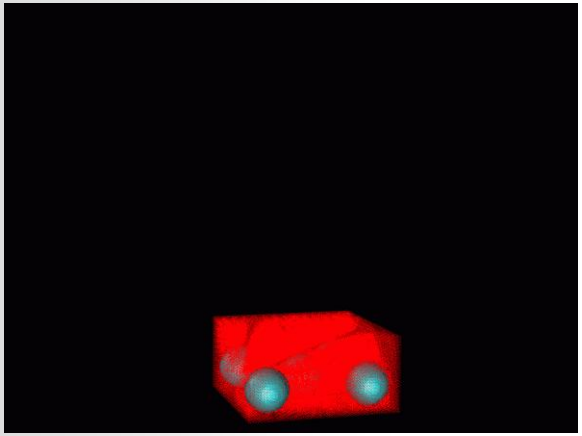
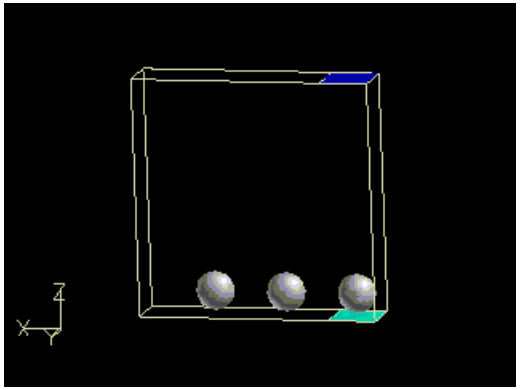
Expanding Capabilities in Modeling Multiphase Flows











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Multiphase models in ANSYS FLUENT

- **Lagrangian Dispersed Phase Model (DPM)**
  - Lagrangian particle/bubble/droplet tracking
- **Dense dispersed phase model (DDPM)**
  - Lagrangian + Eulerian particle/bubble/droplet tracking
- **Volume of Fluid model (VOF)**
  - Direct method of predicting interface shape between immiscible phases
- **Eulerian Model**
  - Model resulting from averaging of VOF model applicable to a wide range of multiphase flows (primarily used for dispersed flows).
- **Mixture Model**
  - Simplification of Eulerian model
  - Applicable when inertia of dispersed phase is small.
- **Immiscible fluid model**
  - Extension of Eulerian model for direct prediction of interface shape

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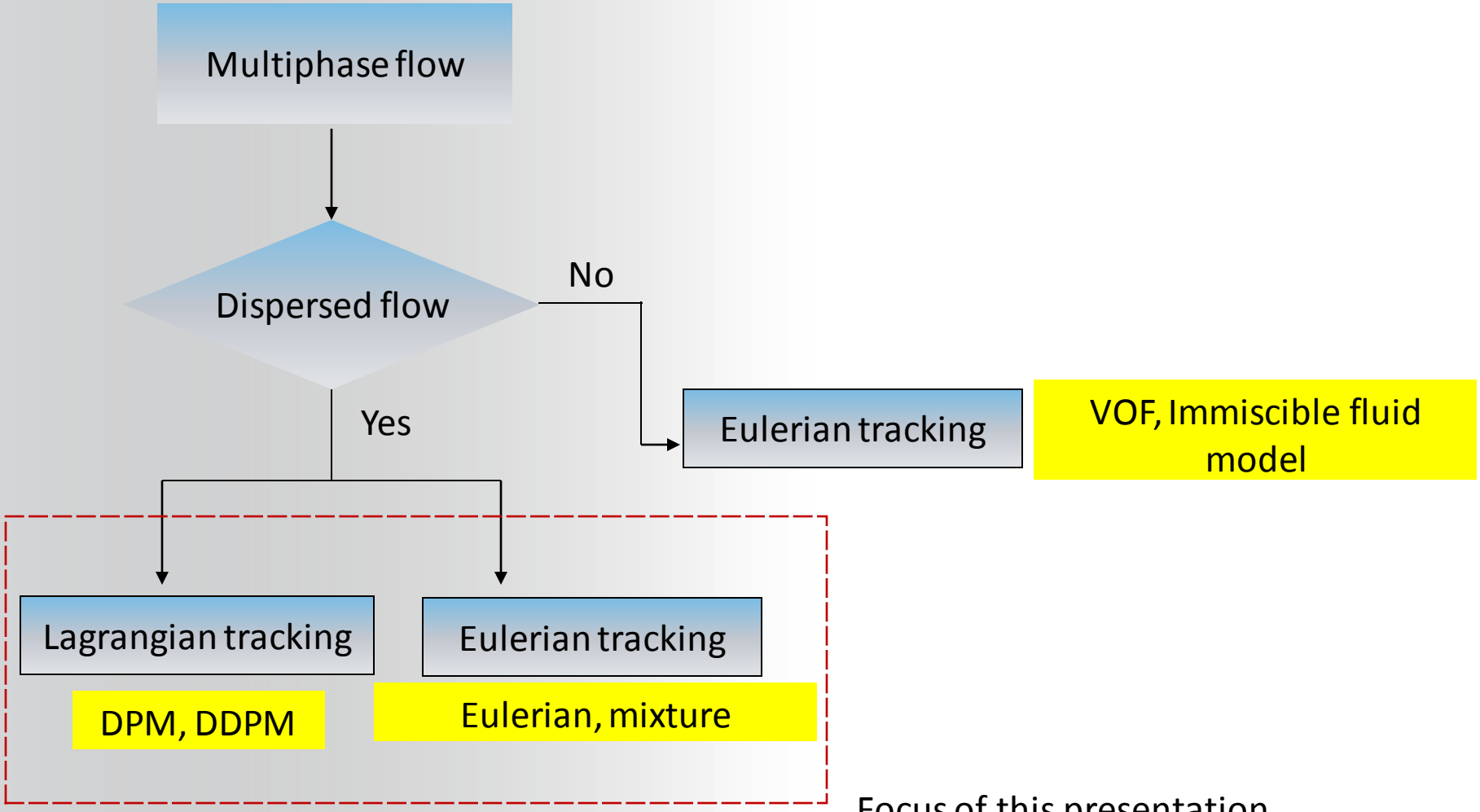
Eulerian vs. Lagrangian tracking



Focus of this presentation

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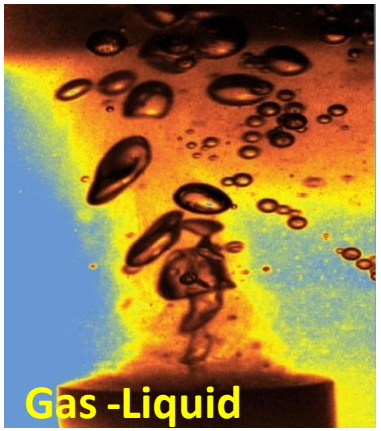
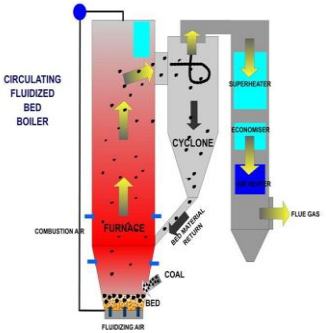
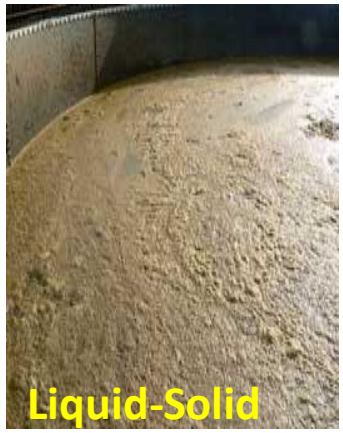
Dispersed Multiphase Flows

- **Range of applicability**
  - Flow regime
    - Bubbly flow, droplet flow, slurry flow,
    - fluidized bed, particle-laden flow
  - Volume loading
    - Dilute to dense
  - Particulate loading
    - Low to high
  - Stokes number
    - All ranges
- **Application examples**
  - Gas-Liquid/Liquid-Liquid
    - Bubble column reactor, emulsion flows
  - Gas-Solid
    - High particle loading flows, Fluidized beds,
    - Riser, cyclone
  - Liquid-Solid
    - Slurry flows, Sedimentation, Packed bed reactors components





Gas-Solid



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Discrete phase model

- The fluid phase is treated as a continuum, while the dispersed phase is solved by tracking a large number of particles, bubbles, or droplets through the calculated flow field.
- The dispersed phase can exchange momentum, mass, and energy with the fluid phase.
- A fundamental assumption made in this model is that the dispersed phase occupies a low volume fraction (>10 %).
  - high mass loading *is acceptable.*
- The model is appropriate for the modelling of spray dryers, coal and liquid combustion, and some particle-laden flows
- It is inappropriate for the modelling of liquid-liquid mixtures, fluidized beds where the volume fraction of the second phase is not negligible.

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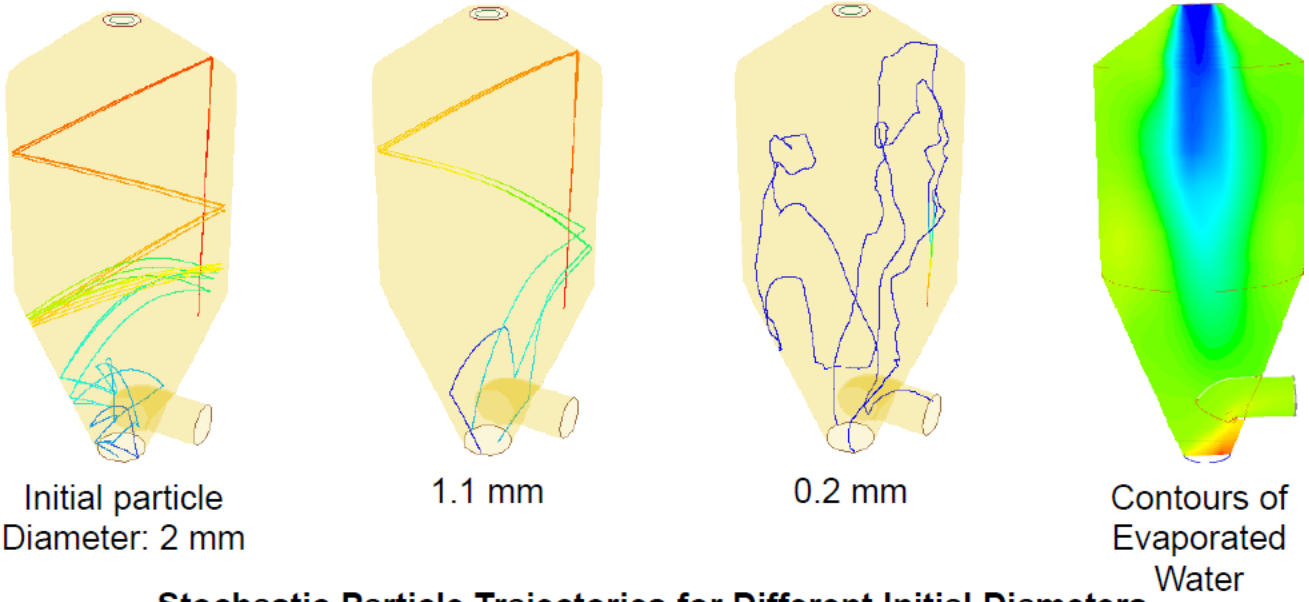
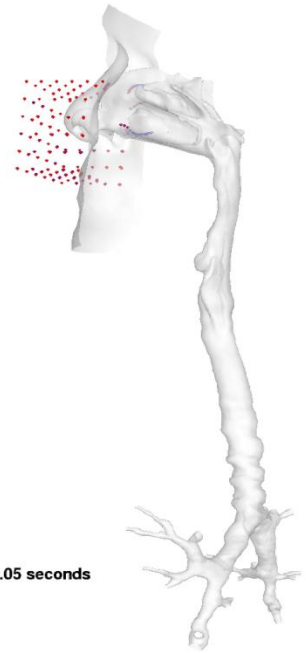
DPM Model Applications



Stochastic Particle Trajectories for Different Initial Diameters

Spray Dryer



Drug Delivery

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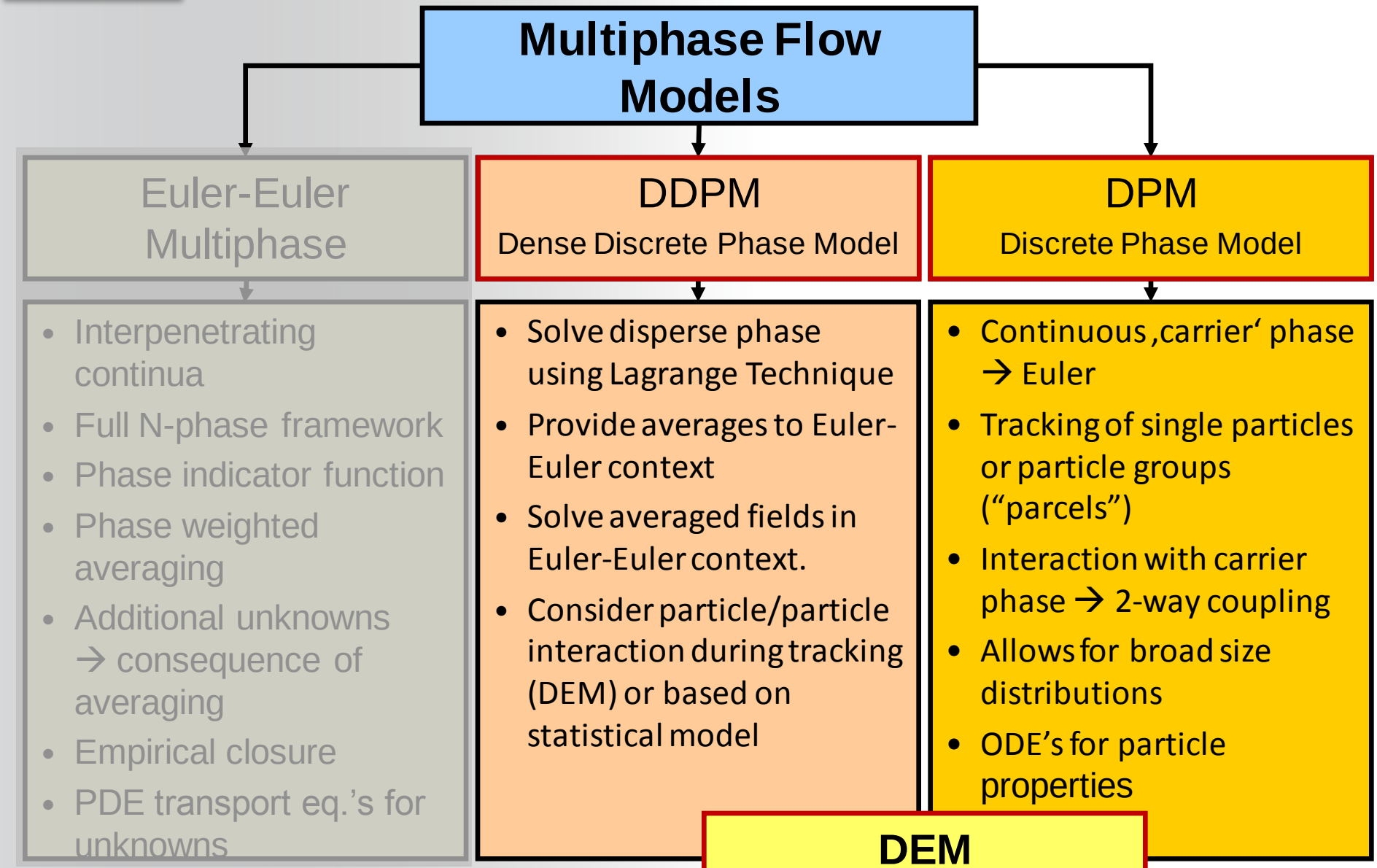
Dense Discrete Phase Model



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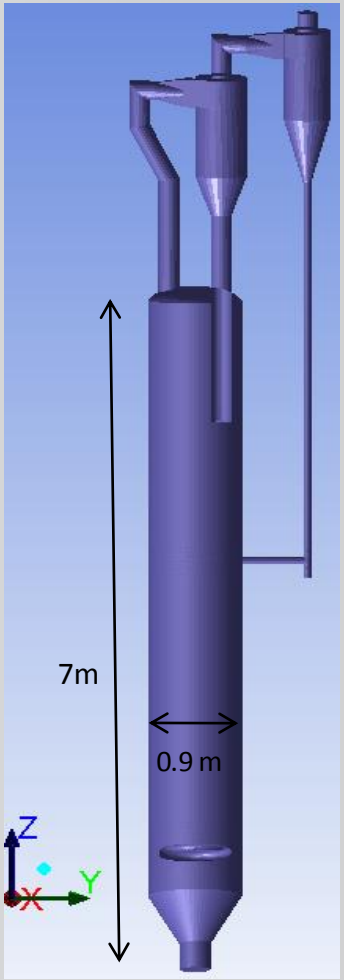
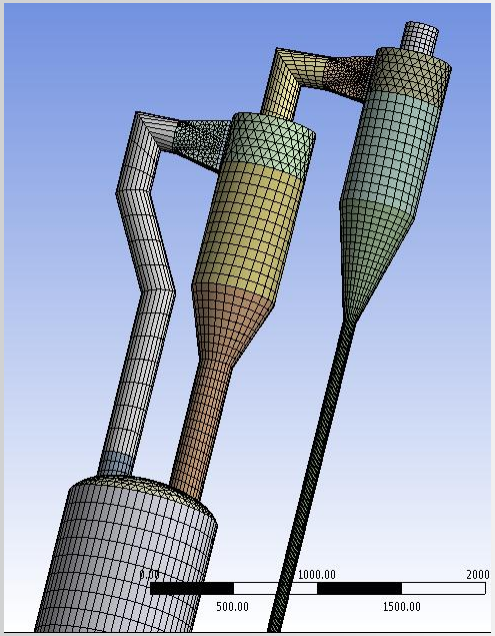
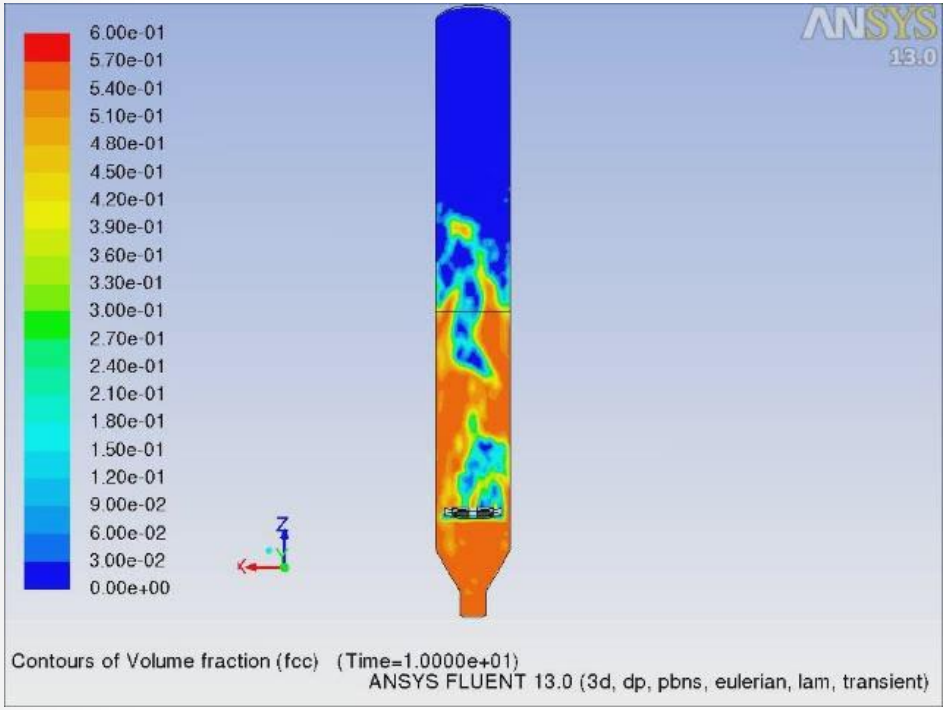
Application of DDPM Model

NETL Fluidization Challenge Problem



Complete Geometry





Kinetic theory based particle-particle interaction

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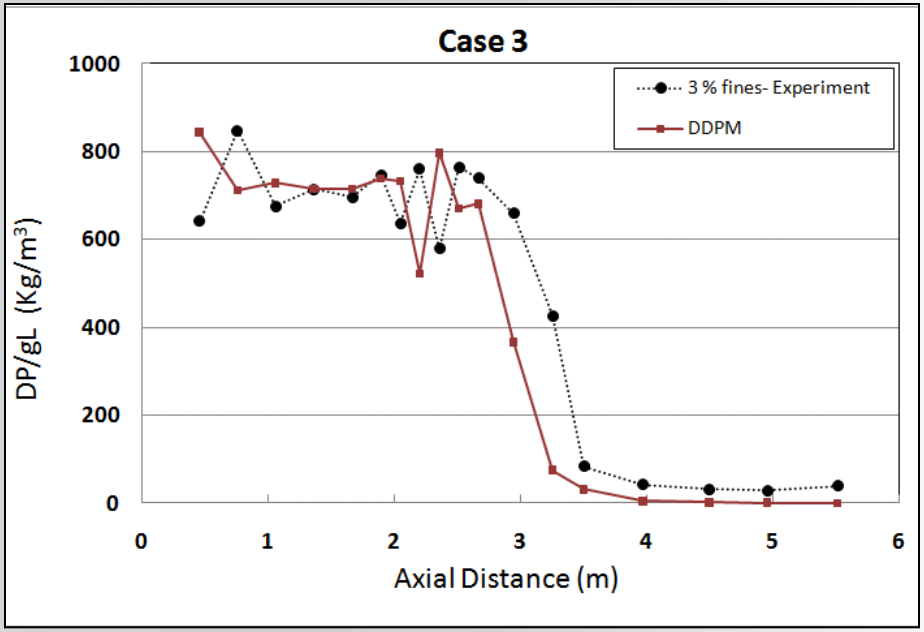
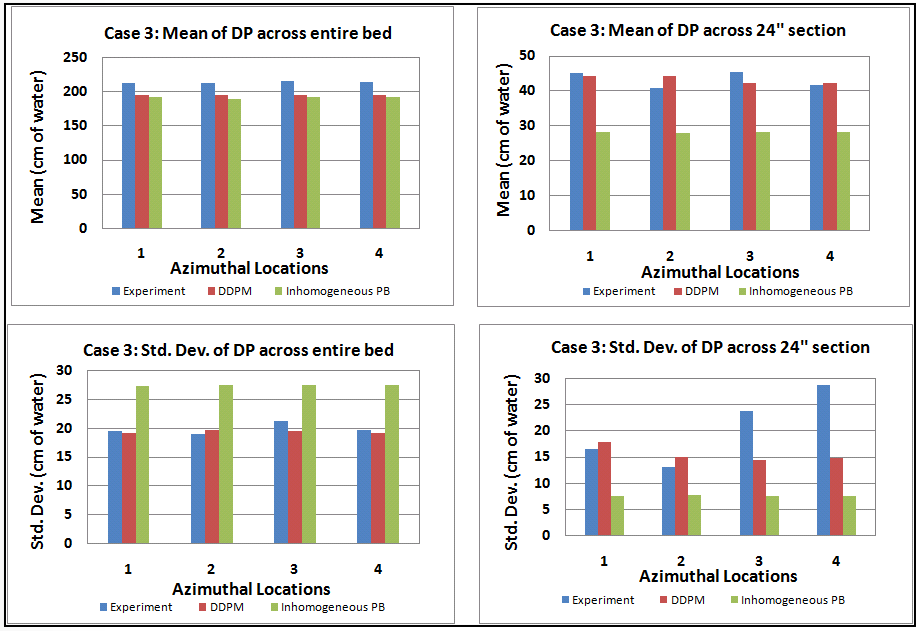
Application of DDPM Model

NETL Fluidization Challenge Problem





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Eulerian Multiphase Model

- In Eulerian Model phases are treated as interpenetrating continua
- Averaging techniques are employed to develop effective conservation equations (mass, momentum and energy) of each phase.
- Conservation equations of different phases are coupled via interaction terms, which are modeled.
  - Drag, virtual mass, lift and other forces
- For Eulerian-Granular model particle phase constitutive relations are obtained from application of kinetic theory of dense gases.
- Applications of the Eulerian multiphase model include bubble columns, risers, particle suspension, and fluidized beds.

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Conservation Equations

- **Continuity:**

Volume fraction for the q^{th} phase

$$\frac{\partial\left(\alpha_q \rho_q\right)}{\partial t}+\nabla\cdot\left(\alpha_q \rho_q \mathbf{u}_q\right)=\sum_{p=1}^{n}\dot{m}_{pq}$$

- **Momentum for q^{th} phase:**

$$\underbrace{\frac{\partial\left(\alpha_q\rho_q\mathbf{u}_q\right)}{\partial t}}_{\text{transient}}+\underbrace{\nabla\cdot\left(\alpha_q \rho_q \mathbf{u}_q \mathbf{u}_q\right)}_{\text{convection}}=\underbrace{-\alpha_q\nabla p}_{\text{pressure}}+\underbrace{\alpha_q \rho_q\mathbf{g}}_{\text{body}}+\underbrace{\nabla\cdot\boldsymbol{\tau}_q}_{\text{shear}}+\underbrace{\sum_{p=1}^{n}\left(\mathbf{R}_{pq}}_{\text{interphase forces exchange}}+\underbrace{\dot{m}_{pq}\mathbf{u}_q\right)}_{\text{interphase mass exchange}}+\underbrace{\alpha_q \rho_q\left(\mathbf{F}_q+\mathbf{F}_{\text{lift},q}+\mathbf{F}_{\text{vm},q}\right)}_{\text{external, lift, and virtual mass forces}}$$

Solids pressure term is included for granular model.

- **The inter-phase exchange forces are expressed as:**

$$\mathbf{R}_{pq}=K_{pq}\left(\mathbf{u}_p-\mathbf{u}_q\right)$$

- **Energy equation for the q^{th} phase can be similarly formulated.**

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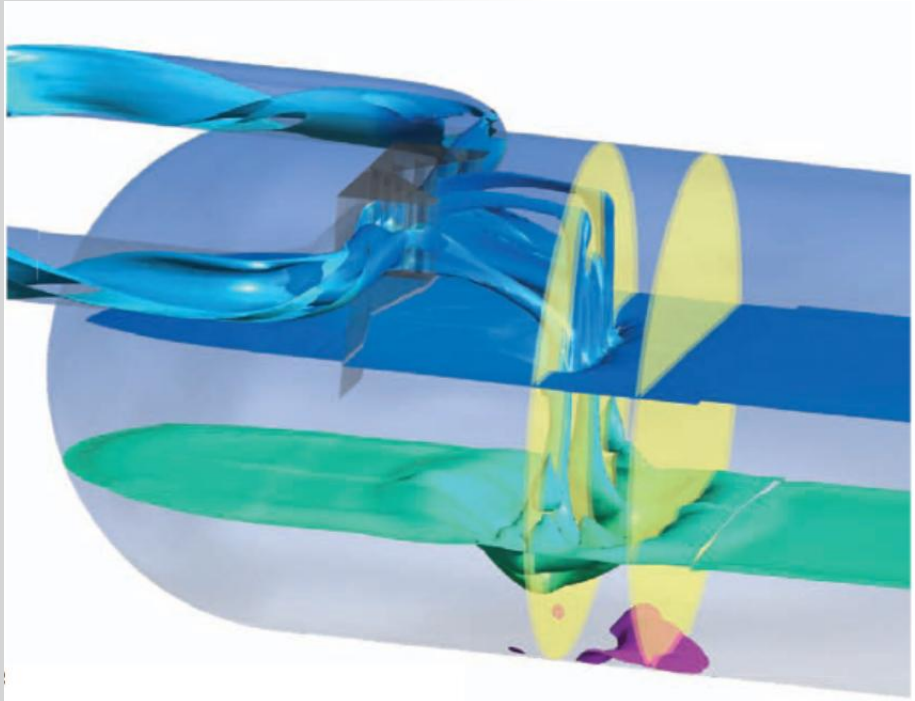
Application of Eulerian Model

Three Phase (oil, gas and water) Separator



Multiphase simulation within a horizontal three-phase separator with inlet piping, a vane-type inlet device and full-diameter perforated baffles. The lower layer of fluid is water; above that is the oil phase with the inlet device in the gas phase of the vessel. The pink area at the bottom of the vessel shows where sand entrained in the water phase will initially settle.

David Stanbridge, Swift Technology Group, Norwich, U.K.
ANSYS Advantage, Volume V, Issue 2, 28-30, 2011

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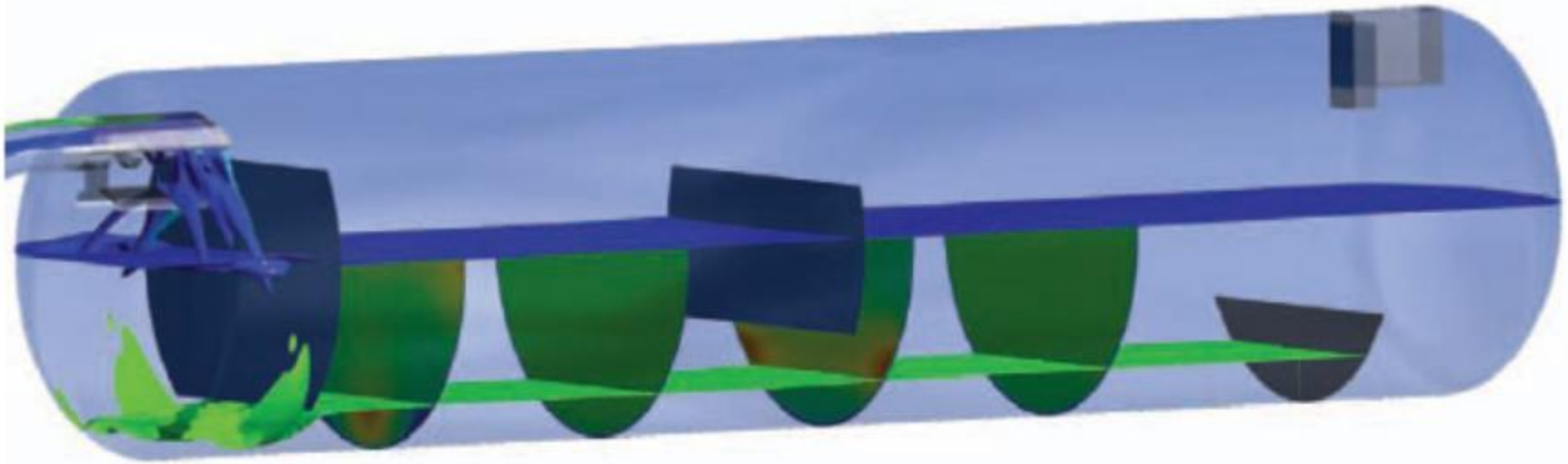
Application of Eulerian Model

Three Phase (oil, gas and water) Separator



The complete length of a typical horizontal separator: The blue layer represents the interface between gas and oil phases, and the green layer represents the interface between oil and water. The vertical blue areas represent part diameter perforated baffles. Along the length of the vessel, four contours show velocity distribution in both oil and water phases.

David Stanbridge, Swift Technology Group, Norwich, U.K.
ANSYS Advantage, Volume V, Issue 2, 28-30, 2011

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Mixture Multiphase Model

- **The mixture model, like the VOF model, uses a single–fluid approach. It differs from the VOF model in two respects:**

– the mixture model allows the phases to be interpenetrating the volume fractions can therefore vary between 0 and 1;

– the mixture model allows the phases to move at different velocities using the concept of slip (or drift) velocities

- **(note that the phases can also be assumed to move at the same velocity and the mixture model is then reduced to a homogeneous multiphase model).**

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Conservation Equations

- **Solves one equation for continuity of mixture**

$$\frac{\partial \rho_m}{\partial t} + \nabla \cdot \left(\rho_m \vec{u}_m \right) = 0$$

- **Solves one equation for the momentum of the mixture**

$$\frac{\partial \left(\rho \vec{u}_m \right)}{\partial t} + \nabla \cdot \left(\rho_m \vec{u}_m \vec{u}_m \right) = -\nabla p + \nabla \left[\mu_{\text{eff}} \left(\nabla \vec{u}_m + \nabla \vec{u}_m{}^T \right) \right] + \rho_m \vec{g} + \vec{F} + \nabla \sum_{k=1}^{n} \alpha_k \rho_k \vec{u}_k^r \vec{u}_k^r$$

- **Solves for the transport of volume fraction of each secondary phase**

$$\frac{\partial}{\partial t} (\alpha_p \rho_p) + \nabla . (\alpha_p \rho_p \vec{u}_m) = -\nabla . (\alpha_p \rho_p \vec{u}_p^r)$$

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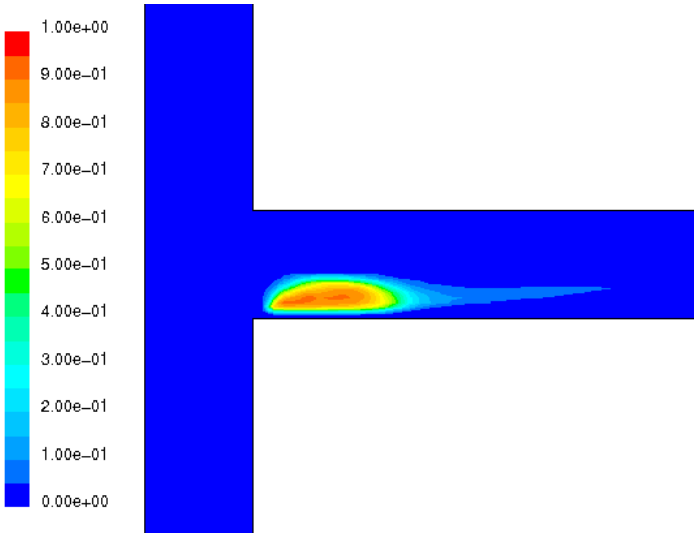
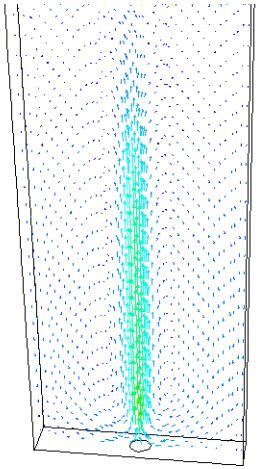
Applications of Mixture Model

- **Non-homogeneous mixture model can be used to describe all phases if the following conditions are satisfied**
  - No countercurrent flow
- **Applicable to low particle relaxation times**

$$\tau_p = \frac{\rho_p d_p^2}{18\mu_f} < \frac{D}{U}$$

- **One continuous phase and N dispersed phases**
- **Limitations can be overcome via UDF for relative velocity**





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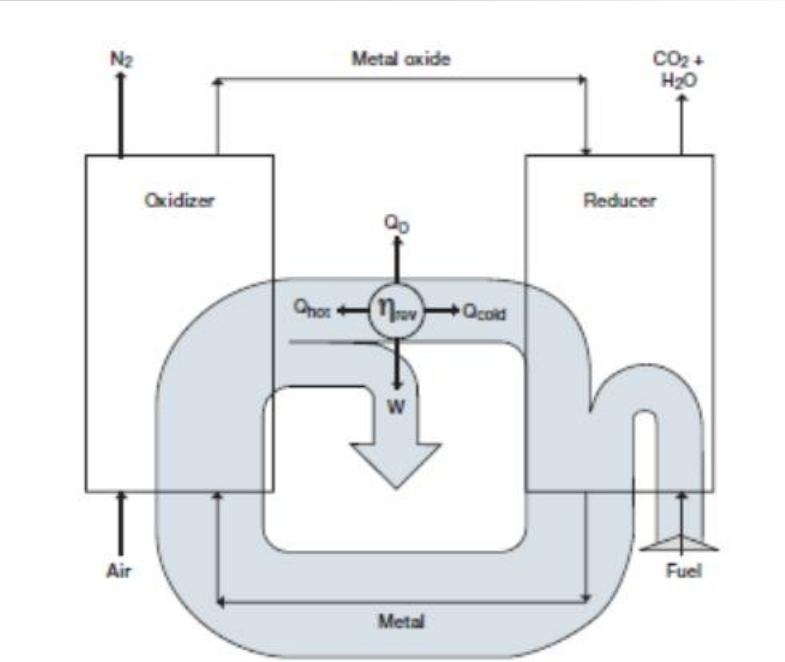
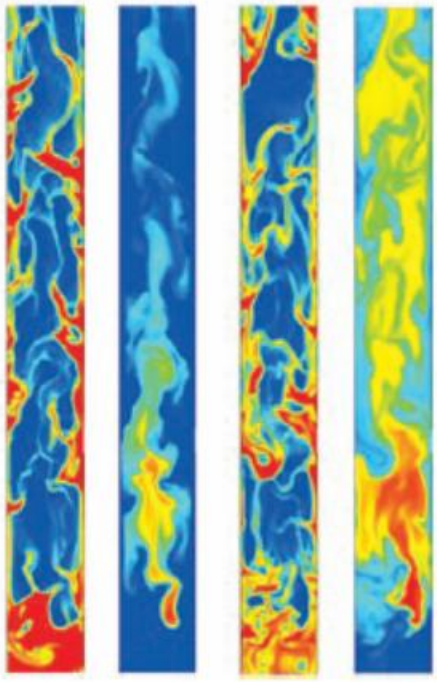
Applications of Eulerian-Granular Model

Chemical Looping Combustion



Chemical-looping combustion process



The interaction between particle clusters and reacting gas using a particle with high reactivity (two images on the left) and low reactivity (two images on the right). In each pair of images, the one on the left shows the particle volume fraction, and the one on the right shows the reacting gas concentration.

Schalk Cloete and Shahriar Amini, Flow Technology Research Group, SINTEF Materials and Chemistry, Trondheim, Norway
ANSYS Advantage, Volume V, Issue 1, 15-16, 2011

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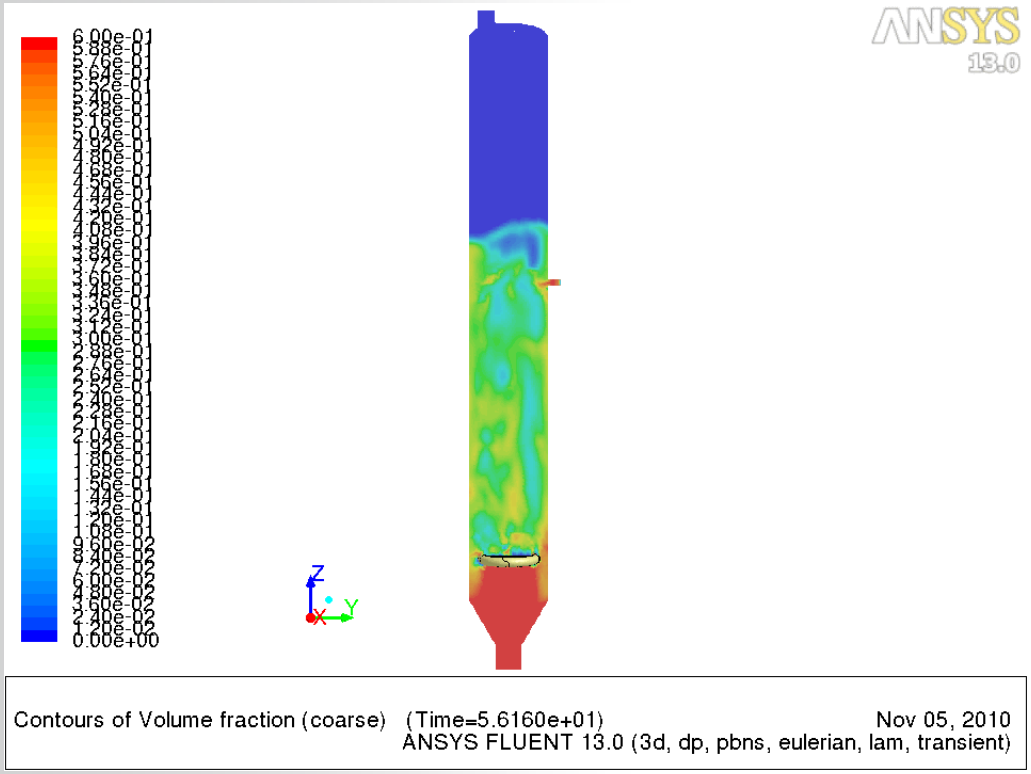
Applications of Eulerian-Granular Model

NETL Fluidization Challenge Problem



Eulerian-Granular model with in-homogeneous discrete population balance method to account for PSD (Particle Size Distribution), aggregation and breakage.

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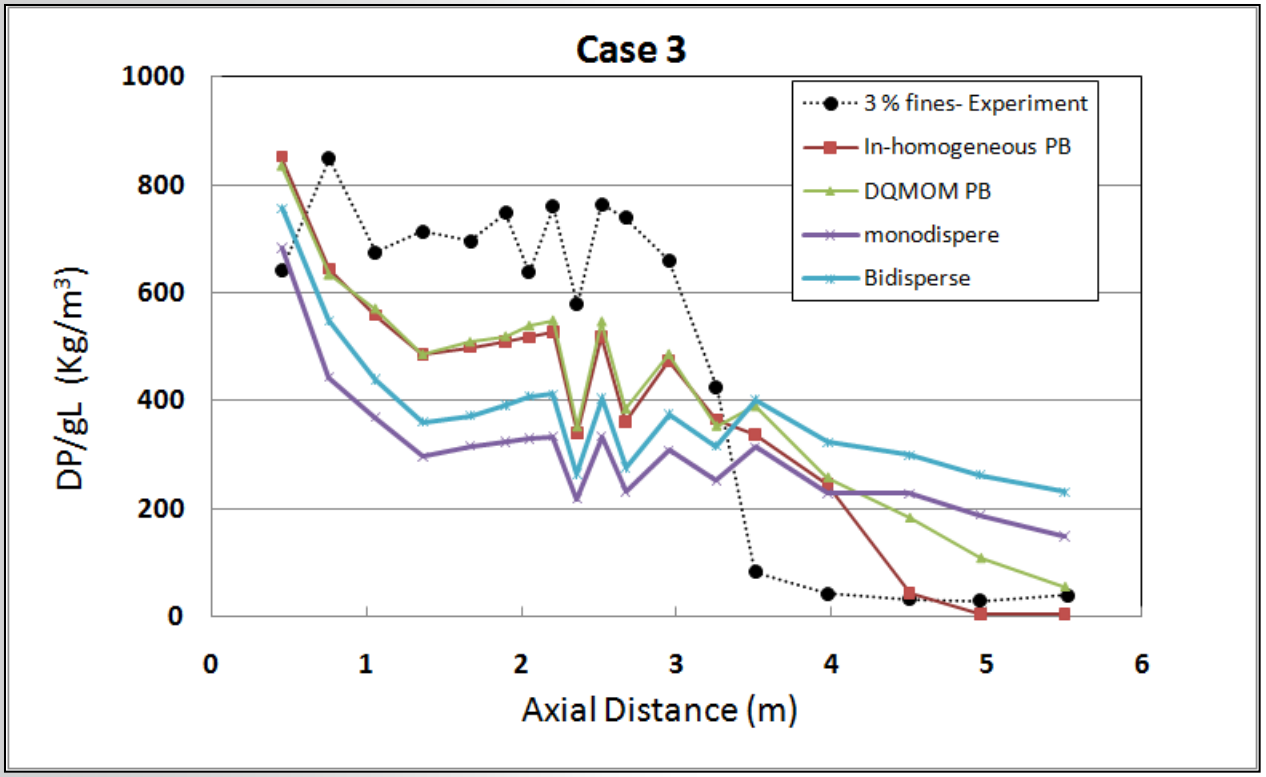
NETL Fluidization Challenge Problem



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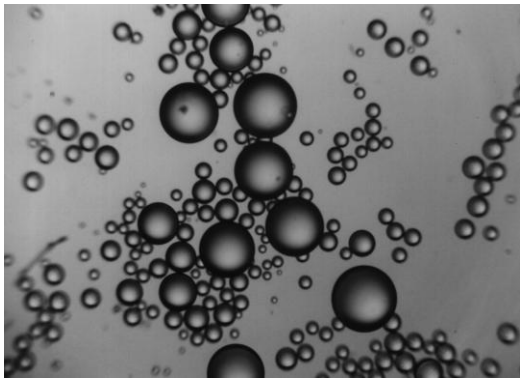
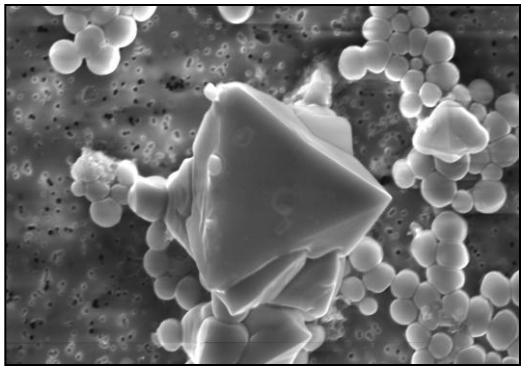
Population Balance Model (PBM)

- **PBM is the most comprehensive model to simulate particle size distributions.**
- **Includes solution of additional equations which describe particle size evolution due to coalescence, breakup, nucleation and mass change phenomena.**
- **Accuracy of the model depends on the kernels used to model size evolution.**





Applications:

Processes where particle size distribution play an important role

Solid-liquid dispersions: Crystallization, granulation, precipitation

Gas-liquid dispersions : Bubble columns, gas-sparged reactors

Gas-solid dispersions : Fluidized bed reactors (catalytic reactors), polymerization

Liquid-liquid dispersions : Emulsions, High shear mixers, Liquid-liquid separation equipment

Aerosols and hydrosols , Microbial cell populations

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Population Balance Model (PBM)

- **Solution Methods**
  - **Discretized Population Equation**

    This method discretize the particle population into a finite set of size intervals
  - **Method of moments**

    This method transforms the population balance equation to reduce its dimensionality to that of a transport equation for the moments of the number density
    - Standard Method of Moments
    - Quadrature Method of Moments
    - Direct Quadrature Method of Moments

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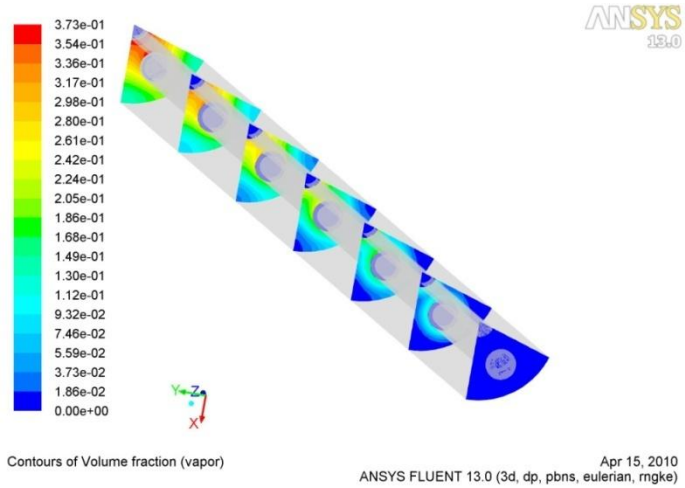
Boiling Models

- **Three boiling model options are available:**
  - **RPI Boiling model**
  - Applicable to subcooled nucleate boiling
  - **Non-equilibrium Boiling**
  - Extension of RPI to take care of saturated boiling
  - **Critical Heat Flux**
  - Extension of RPI to take care of boiling crisis
- **Bubble Diameter:**
  - Algebraic formulations and UDF options
- **Interfacial Transfer models include:**
  - A range of sub-models for *drag and lift*, and turbulent dispersion
  - Liquid/vapor-interface heat and mass transfer models



Contours of vapor volume fraction in a nuclear fuel assembly

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Multiphase Turbulence Modelling

- **Most multiphase turbulence models are simple extension from single phase turbulence closure**
- **Two equation turbulence models available in FLUENT**
  - Mixture model, solves two equation turbulence model based on the mixture of all phases
  - Dispersed model, solves two equation turbulence model for primary phase and assumes turbulence quantities for dispersed phase
  - Full κ–ε model for each individual phase
  - Full k-ω Model for each individual phase
- **Limitations of the eddy viscosity models lead to full stress model in single phase flows: RSM in FLUENT**
  - Full stress model based on the mixture velocity
  - Full stress model for continuous phase with some restrictive assumptions for the turbulence of the dispersed phase and for the exchange term
- **Large Eddy Simulation for the Mixture Multiphase Model**

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Additional Capabilities …

- Species Transport
- Interphase Heat and Mass Transfer
- Homogeneous and Heterogeneous Reactions
- Compatibility with Moving Parts
- Multiphase Flow in Porous Media
- Multiphase with Real Gas
- UDF for “out of box” customization

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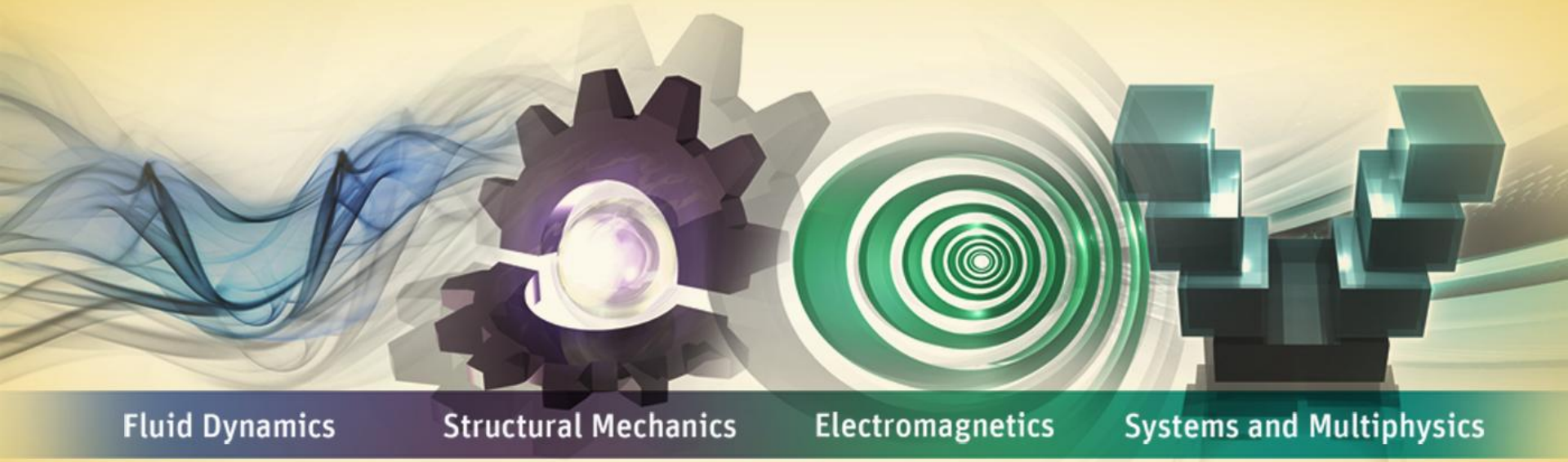
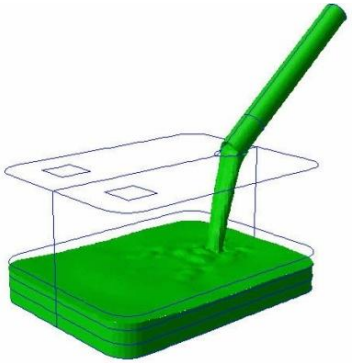
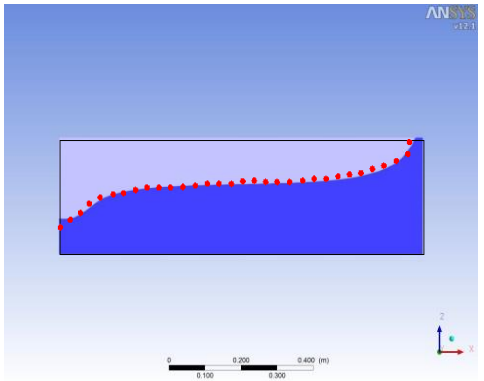
Volume Of Fluid Model In ANSYS CFD

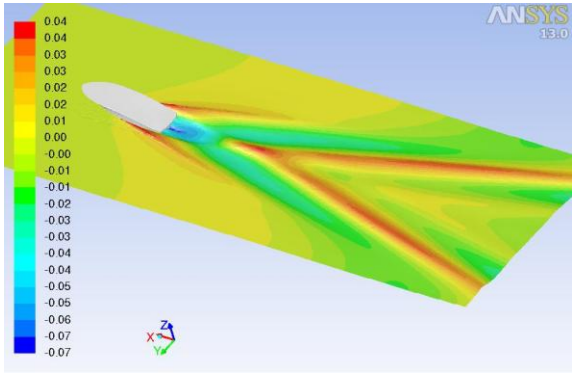


Applicability of the Volume of Fluid Model

- 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 appropriate if interface length is small compared to a computational grid
  - Accuracy of VOF decreases with interface length scale getting closer to the computational grid scale
- Typical problems:
  - Liquid Sloshing
  - Tank Filling
  - 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







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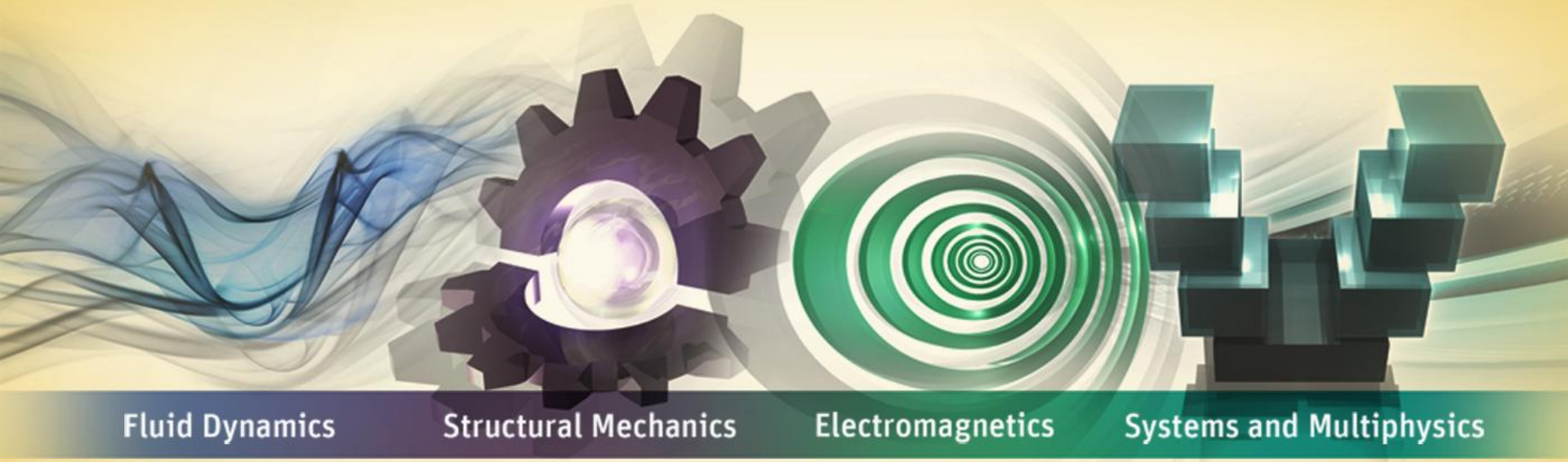
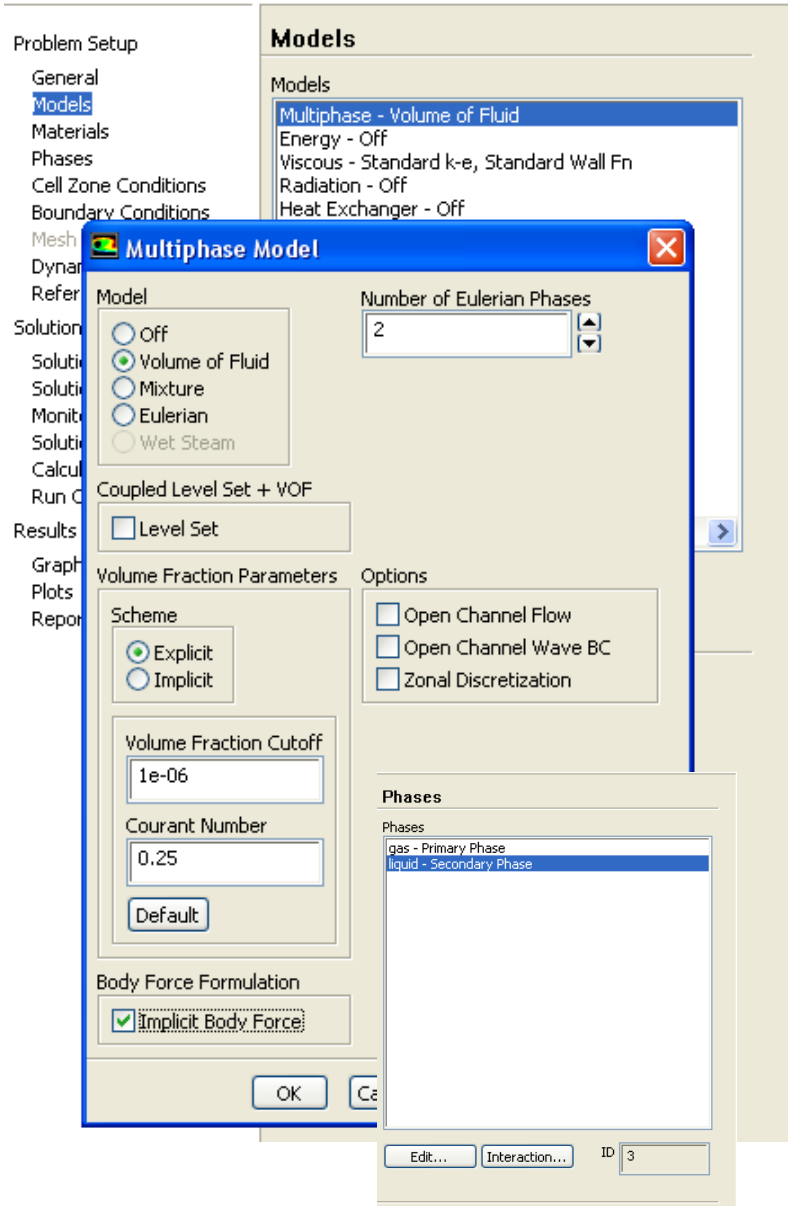
Volume Of Fluid Model In ANSYS FLUENT



Volume of Fluid Model Inputs

- Phases
  - Arbitrary number of phases are allowed
  - Any phase can be primary or secondary – not important in VOF model.
  - Usual practice is to have secondary phase which has less presence in the domain
  - Three ways phases may interact in VOF:
    - Mass exchange
    - Heterogeneous reactions
    - Surface tension with optional wall adhesion effect
- VOF Scheme
  - Explicit and Implicit
  - Controls how phase continuity (volume fraction through which interface is tracked) equation is solved
- Implicit body force (Designed for flows with large body forces)
  - Gravity acting on phases with large density difference.
  - Flows with large rotational accelerations (such as centrifugal separators and/or rotating machinery).
  - The force is handled in robust numerical manner.



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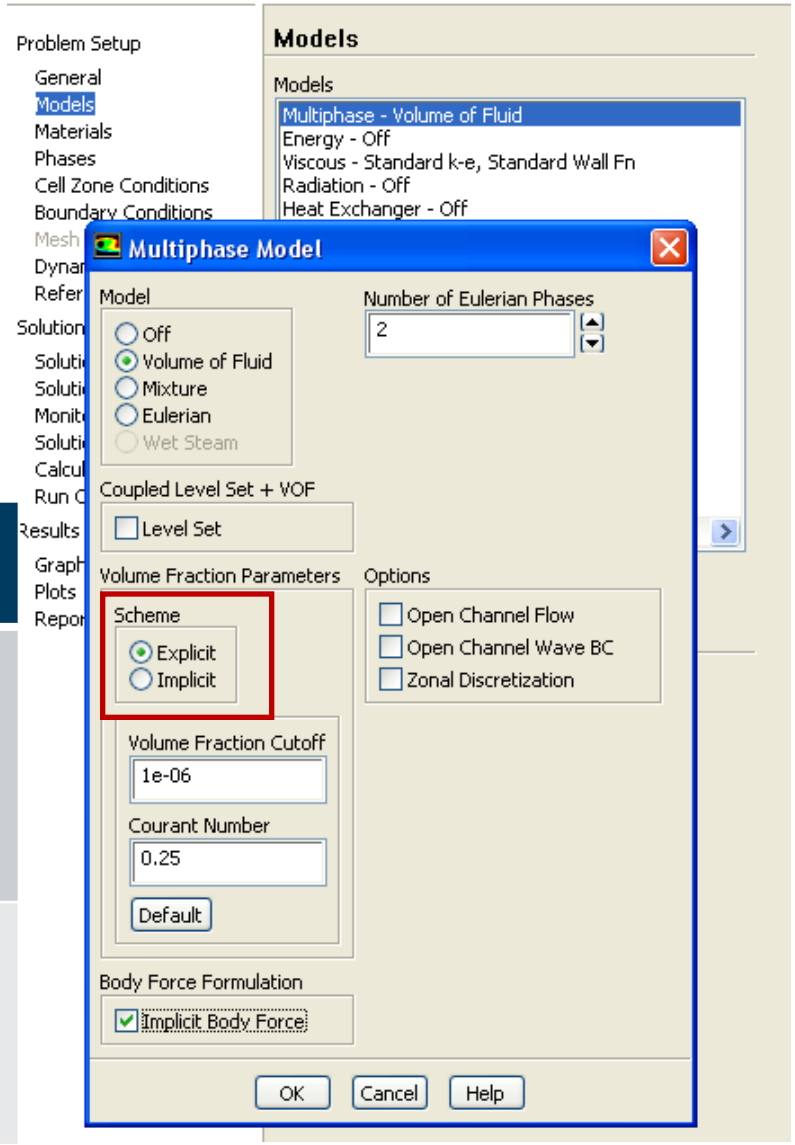
Volume of Fluid Model Schemes

- Explicit Scheme
  - Default and used only with unsteady simulation
  - Explicit scheme solves the volume fraction 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.
- Implicit Scheme
  - Implicit scheme solves phase continuity equation (volume fraction) iteratively together with momentum and pressure.
  - Available with both steady and unsteady simulation

	Advantages	Disadvantages
Explicit VOF	Allows use of Geo-Reconstruct scheme (scheme which renders a sharp interface without numerical diffusion). Should be used in simulation of flows where surface tension is important because of highly accurate curvature calculation.	Poor convergence for skewed meshes. Poor convergence if phases are compressible
Implicit VOF	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 flows)	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



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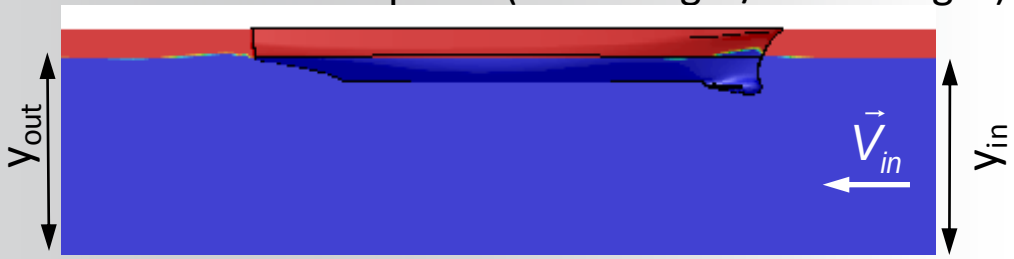
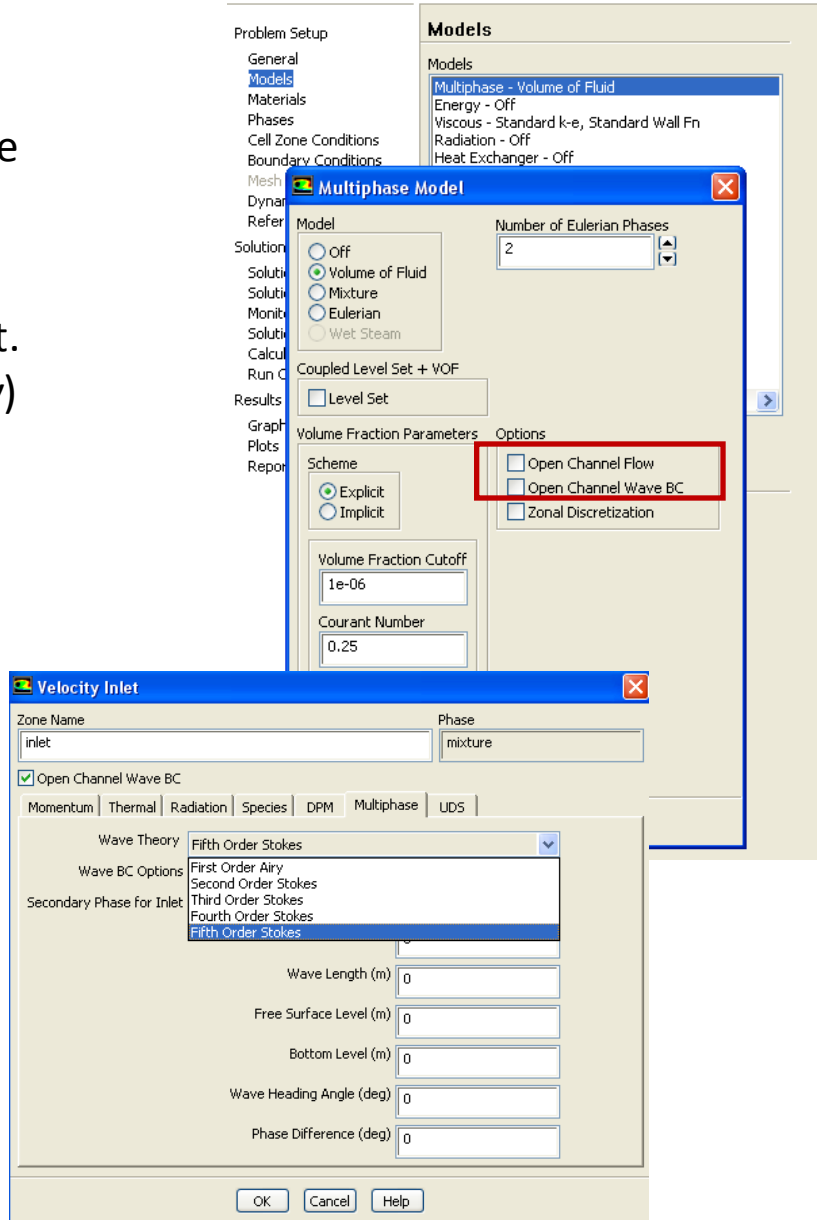
Open Channel Flows

- Open Channel Flow
  - 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 yin and Vin at inlet and y_{out} at the outlet.
  - Characterized by Froude Number , Fr = $V/\sqrt{g\,y}$

- Open Channel Wave BC
  - First order or linear wave theory is applicable for shallow to deep liquid depth ranges
  - Higher order or non-linear wave theories are applicable for intermediate to deep liquid depth range.
  - Choice of Wave theory (within wave breaking limit)
    - Wave theories should be chosen in accordance with wave steepness (wave height/ wave length)





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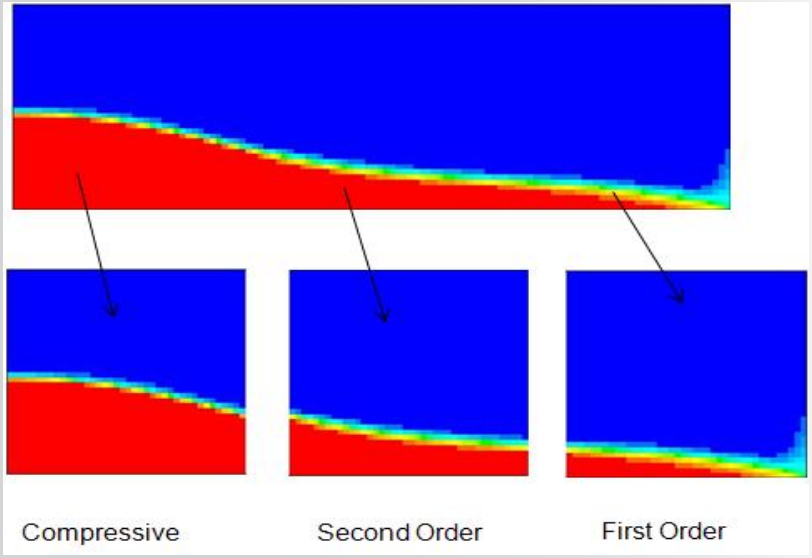
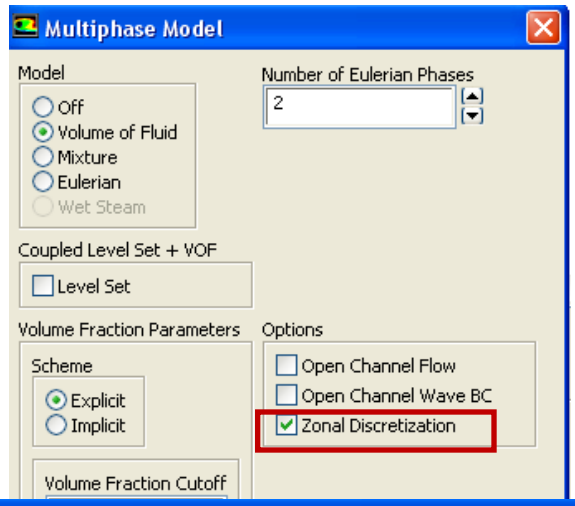
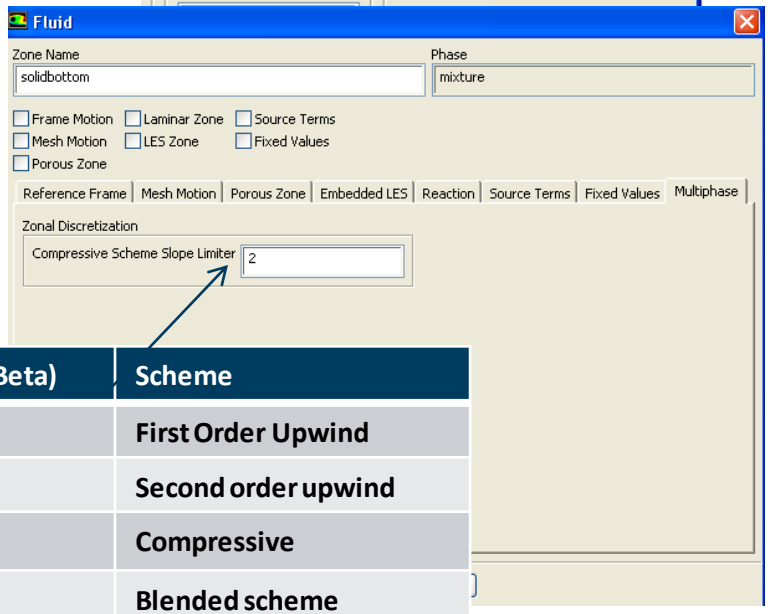
Zonal Discretization

- Zonal Discretization Option
  - This option provides diffusive or sharp interface modeling in different fluid (cell)zones based on the value of zone dependent slope limiter.



(Zone 1) (Zone 2) (Zone 3)





Slope Limiter (Beta)	Scheme
Beta = 0	First Order Upwind
Beta = 1	Second order upwind
Beta = 2	Compressive
0 < Beta < 1 , 1 < Beta < 2	Blended scheme

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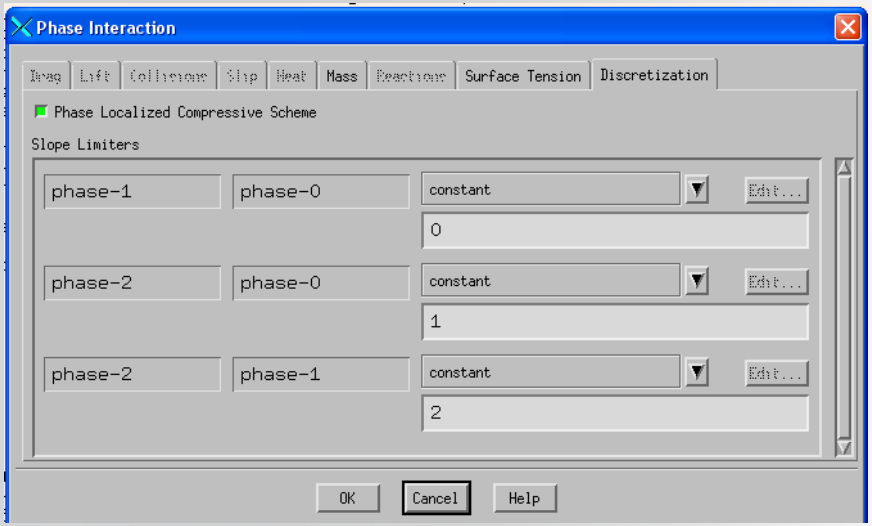
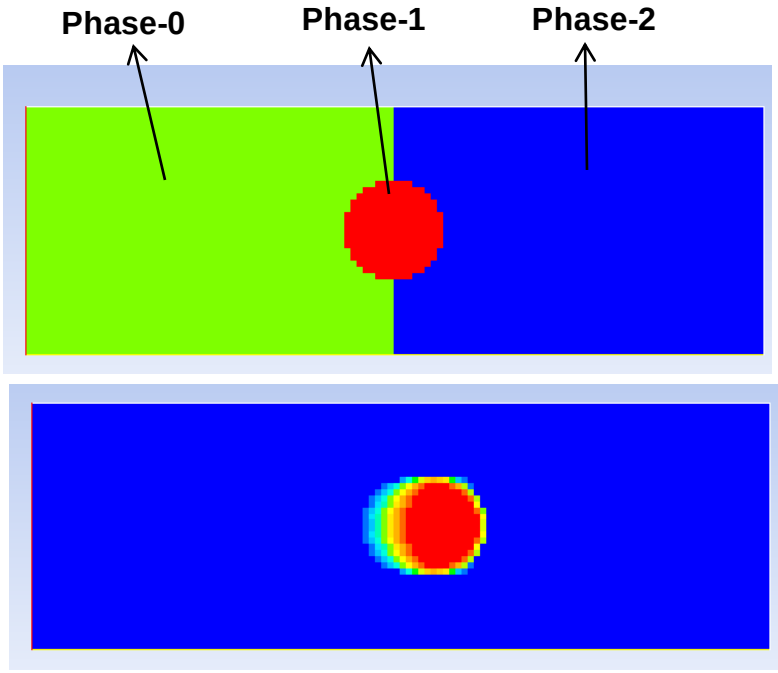
Phase localized Compressive Scheme

- Phase localized compressive scheme facilitates diffusive and sharp modeling of distinct interfaces.
- Phase based discretization is based on effective slope limiter in interfacial cells, where slope limiter is taken as interfacial property between phases.
- Could be effectively used for the cases where HRIC/Compressive schemes produce undesirable behavior.
- It is available with VOF model and Eulerian multiphase using “immiscible fluid model” option.





“Phase localized compressive scheme” with all slope limiters = 2, is same as “Compressive” scheme.

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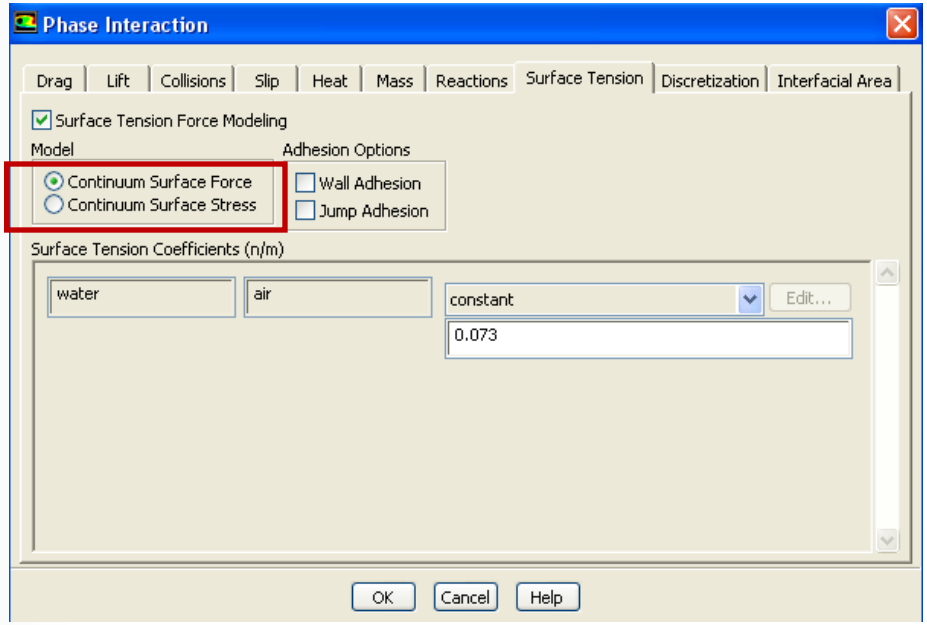
Surface Tension

- CSF
  - In Continuum Surface Force (CSF), the surface curvature is computed from local gradients in the surface normal at the interface.

- CCS
  - New in R 14.0
  - Continuum Surface Stress (CSS) method is alternative way to model surface tension in conservative manner, unlike non-conservative formulation done in CSF method.
  - This method avoids explicit calculation of curvature, and could be represented as anisotropic variant of modeling capillary forces based on surface stresses.
  - CSS method provides few added advantages compared to CSF method, especially for cases involving variable surface tension. However, both CSS and CSF methods introduce parasitic currents at the interface due to imbalance of pressure gradient and surface tension force.
  - Feature supported for only node based smoothing and node based curvature calculation.



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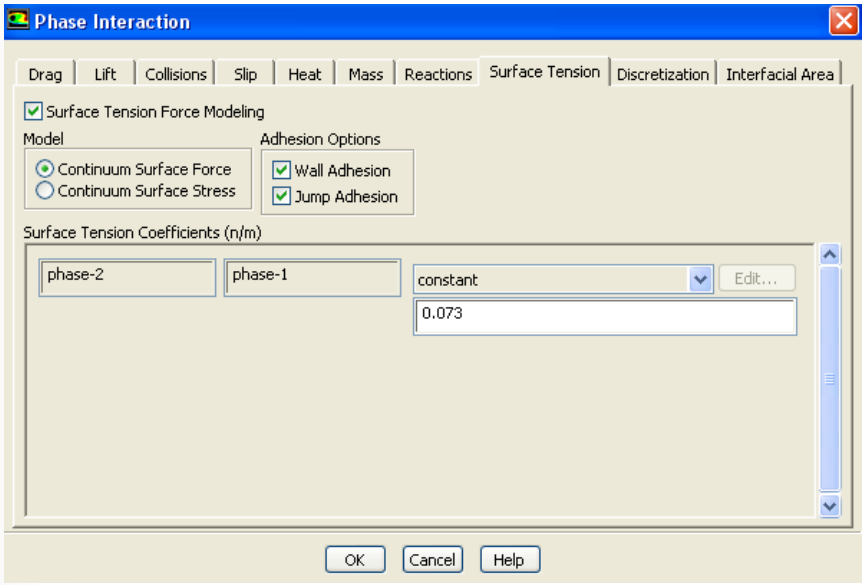
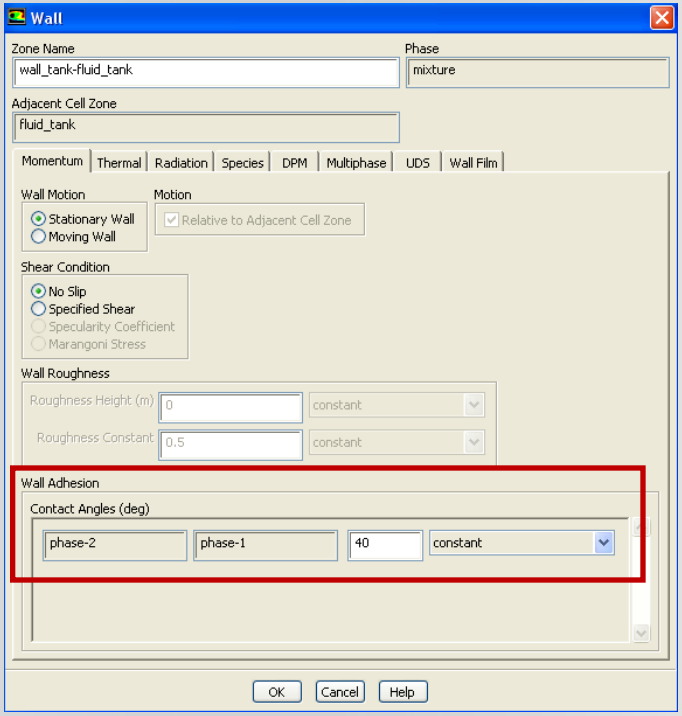
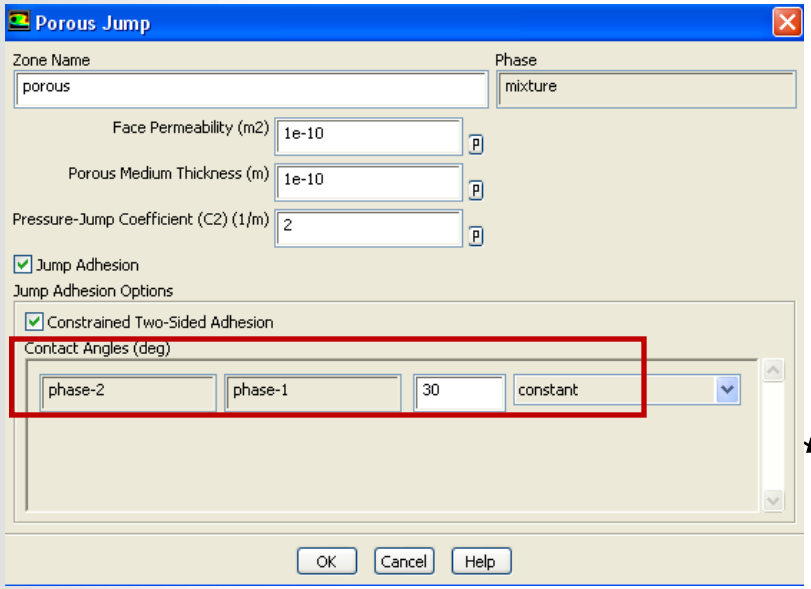
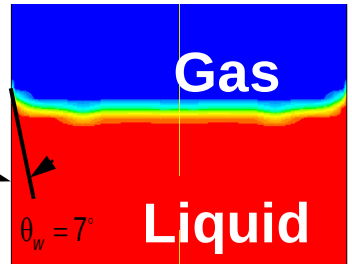
Wall Adhesion

- Wall adhesion
  - Wall adhesion force is a measure of the cohesive forces acting between the fluid and walls.
  - Adhesion is important when modeling meniscus shapes and/or wettability.
  - Jump Adhesion
  - contact angle specification at porous jump boundary









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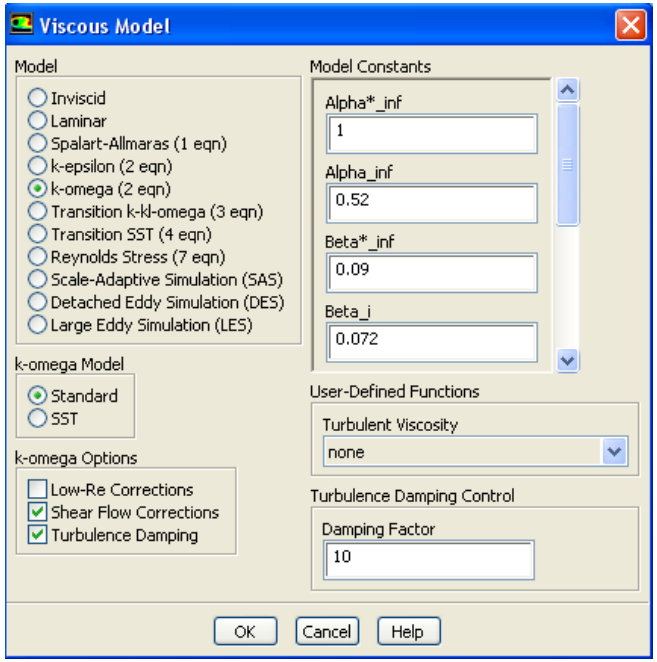
Turbulence Damping

- **Turbulence damping at the interface**
  - **The mesh at the free surface is not fine enough to capture the velocity gradients correctly. The turbulent quantities are over predicted due to this higher velocity gradients.**
  - Turbulence damping helps in getting correct profiles with coarse meshes
- **This treatment is available only for k-omega turbulence model**
- **Source term is added for the omega equation in the interfacial cells which enforces the high value of omega and thus produces turbulence damping.**



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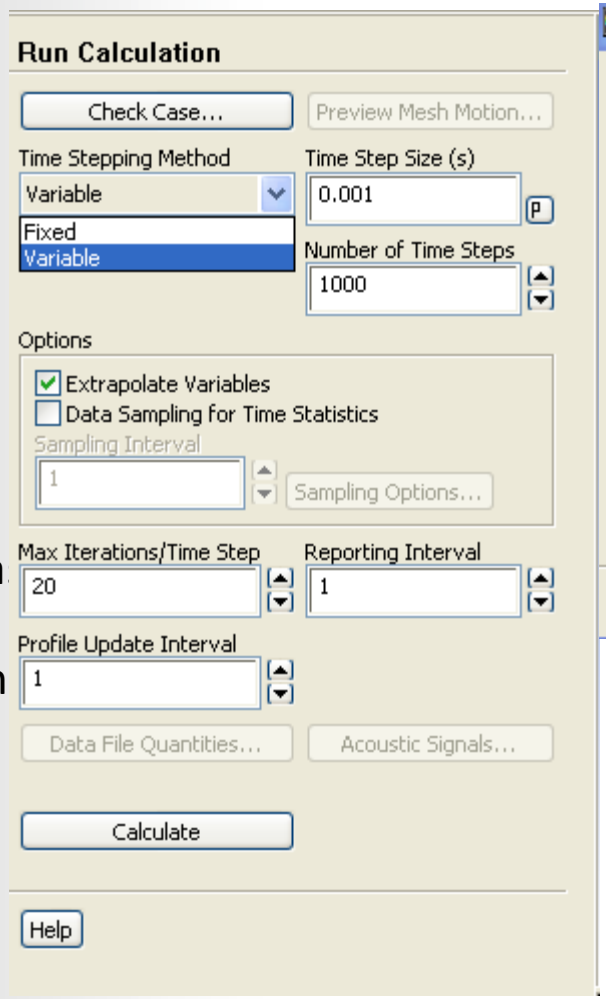
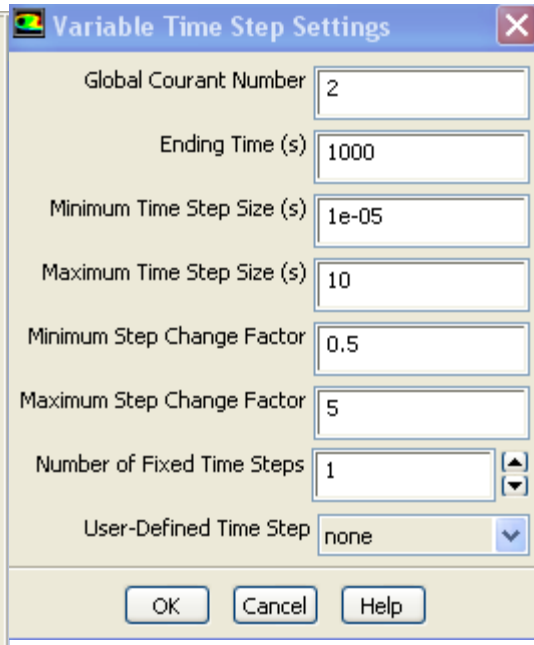
Variable Time Stepping With Explicit VOF

- Variable time stepping
- Scheme for explicit VOF
- Automatically adjusts the time step based on
  - Global Courant number
- Controls can be provided for
  - Max and min time steps used
  - Change factor for time steps
- It is useful for explicit problems a the time step determines the stability for speed of the solution





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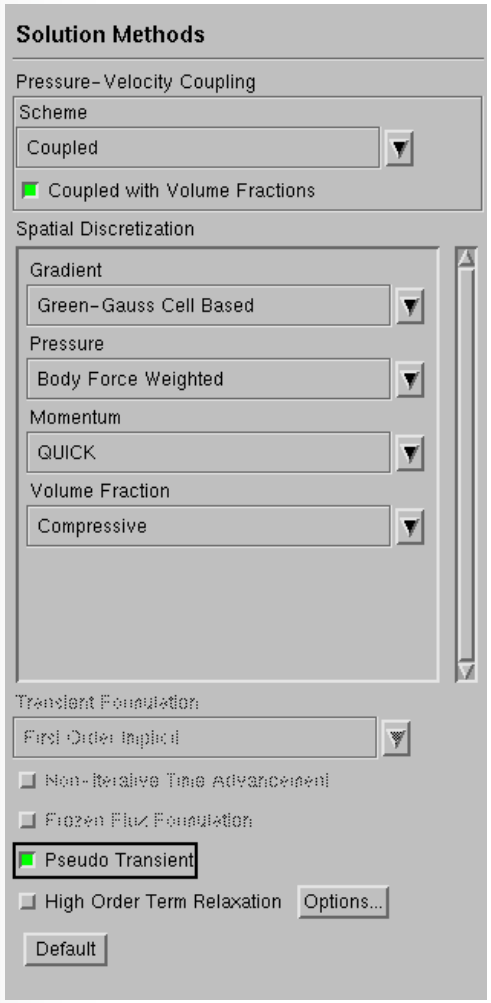
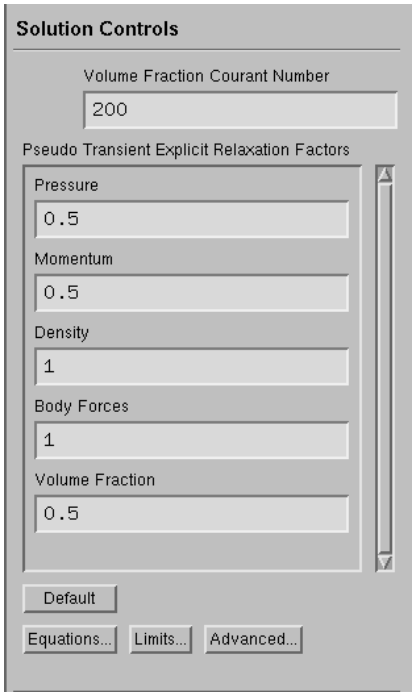
Coupled VOF Solver

- Solves the momentum, pressure based continuity and volume fraction equations together.
- The full implicit coupling achieved through an implicit discretization of pressure gradient terms in the momentum equation and implicit discretization of face mass flux in continuity and volume fraction equations.
- Formulation involves the following linearization
- Linearization of phase mass flux in VOF equation
- Linearization of body force due to gravity in momentum equation
- Coupled VOF solver aims to achieve faster steady state solution compared to segregated method of solving equations.





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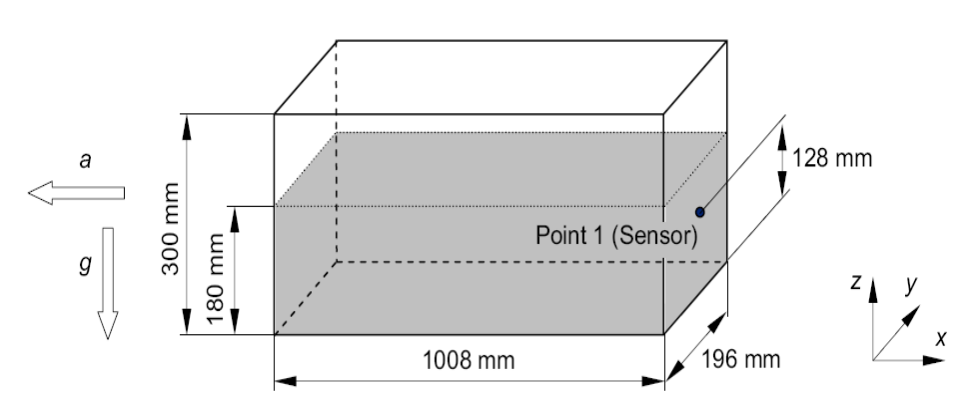
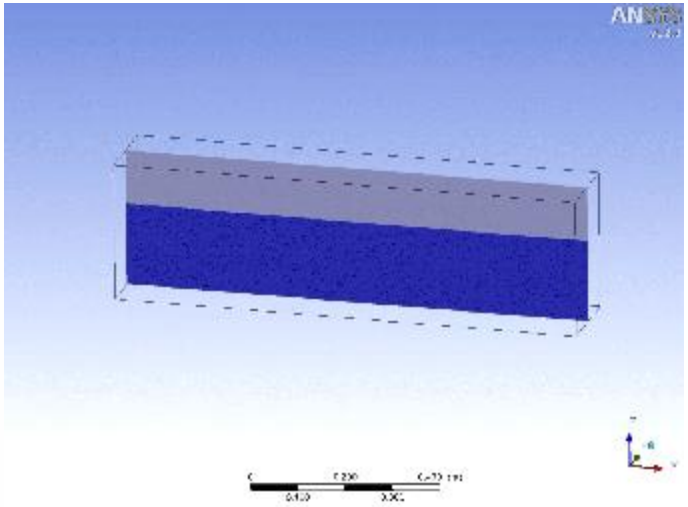
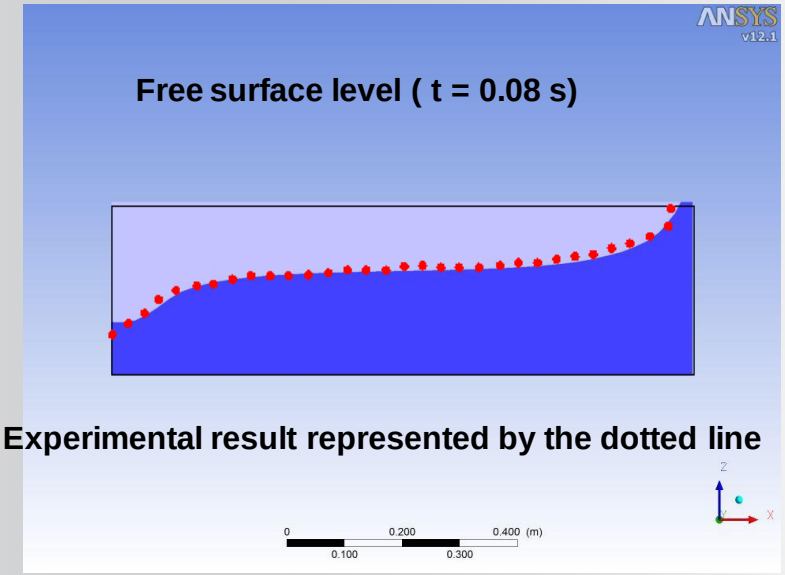
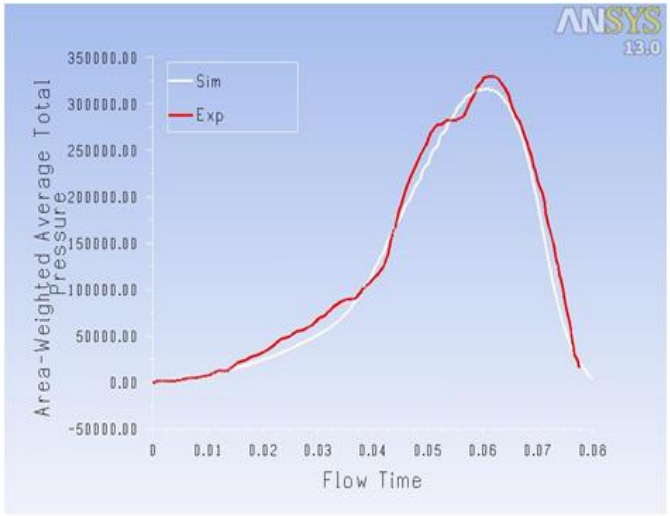
Sloshing



Reference : Simulation of Fuel Sloshing- Comparative Study, Matej Vesenjek, Heiner Mullerschon, Alexander Hummel, Zoran Ren,







Plots for total pressure vs time at a point-1 (comparison with experiment)

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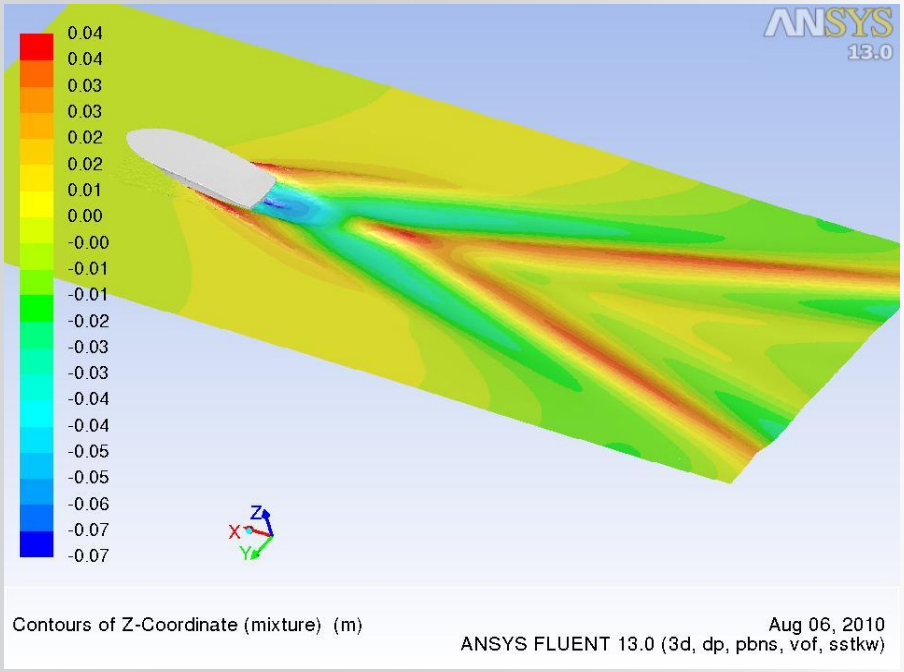
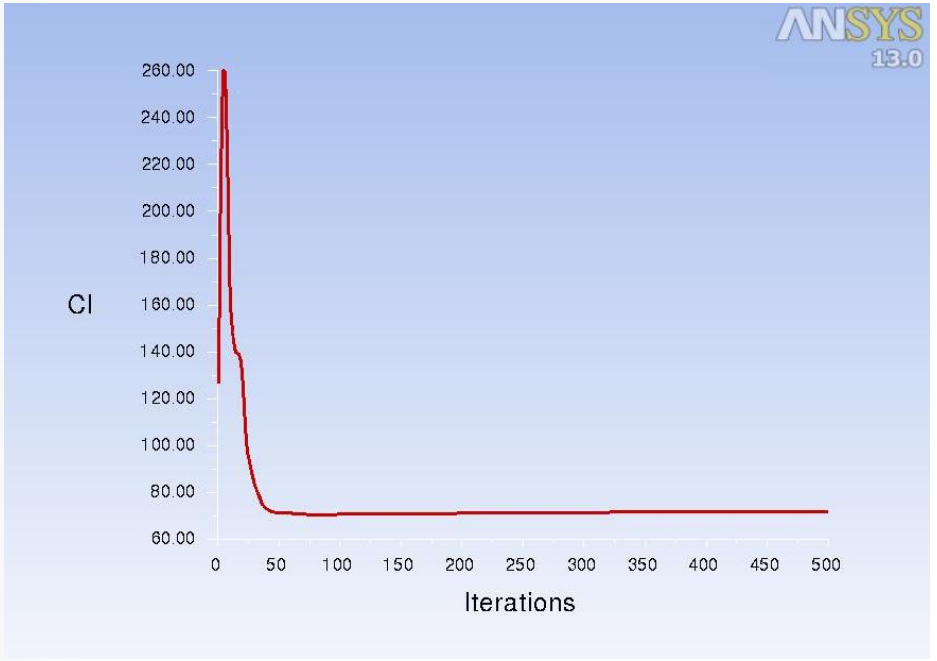
Planning Hull Simulation

Free surface wave elevation contour



Lift Convergence



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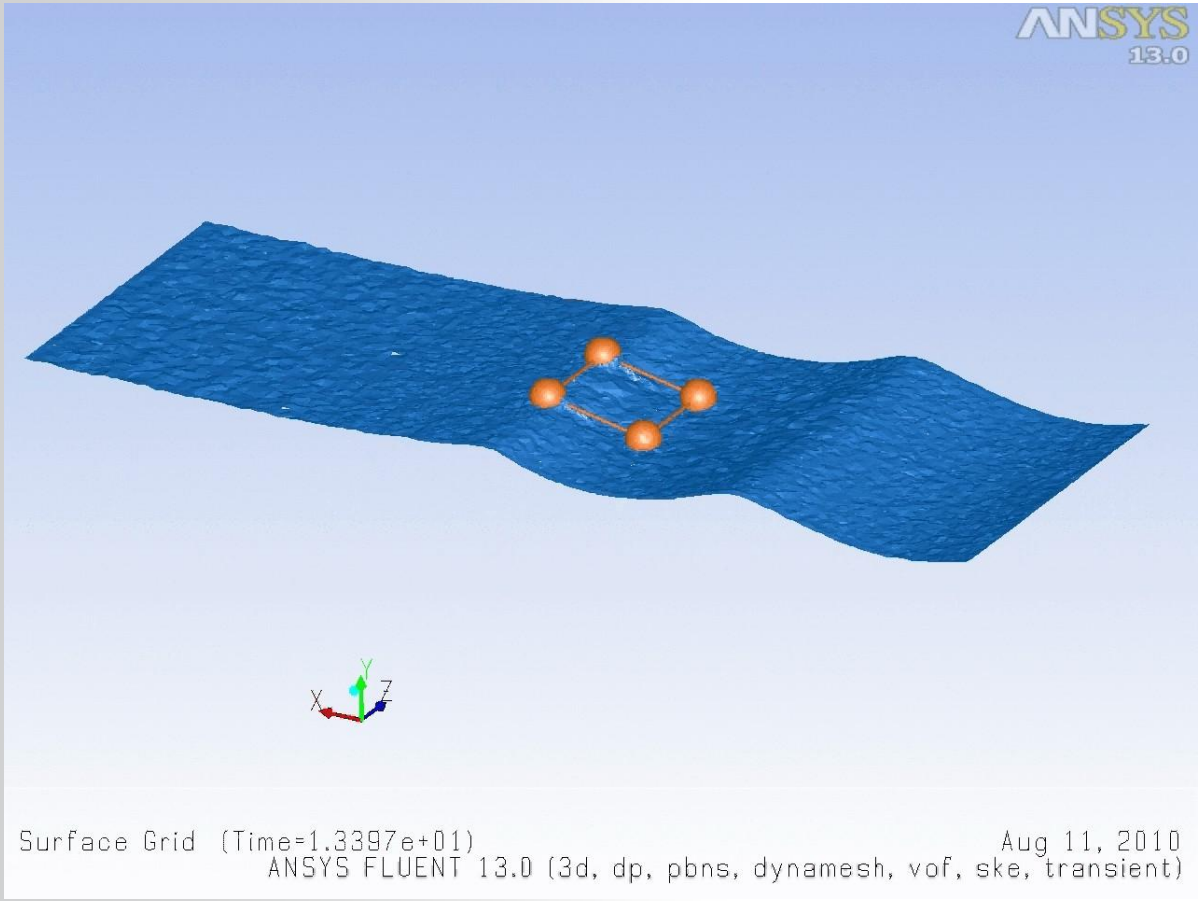
Wave Interaction With A Floating Structure

- **MDM (Moving Deforming Mesh), 6DOF (6 Degrees of Freedom)and Open** channel Wave BC **along with VOF model was used**



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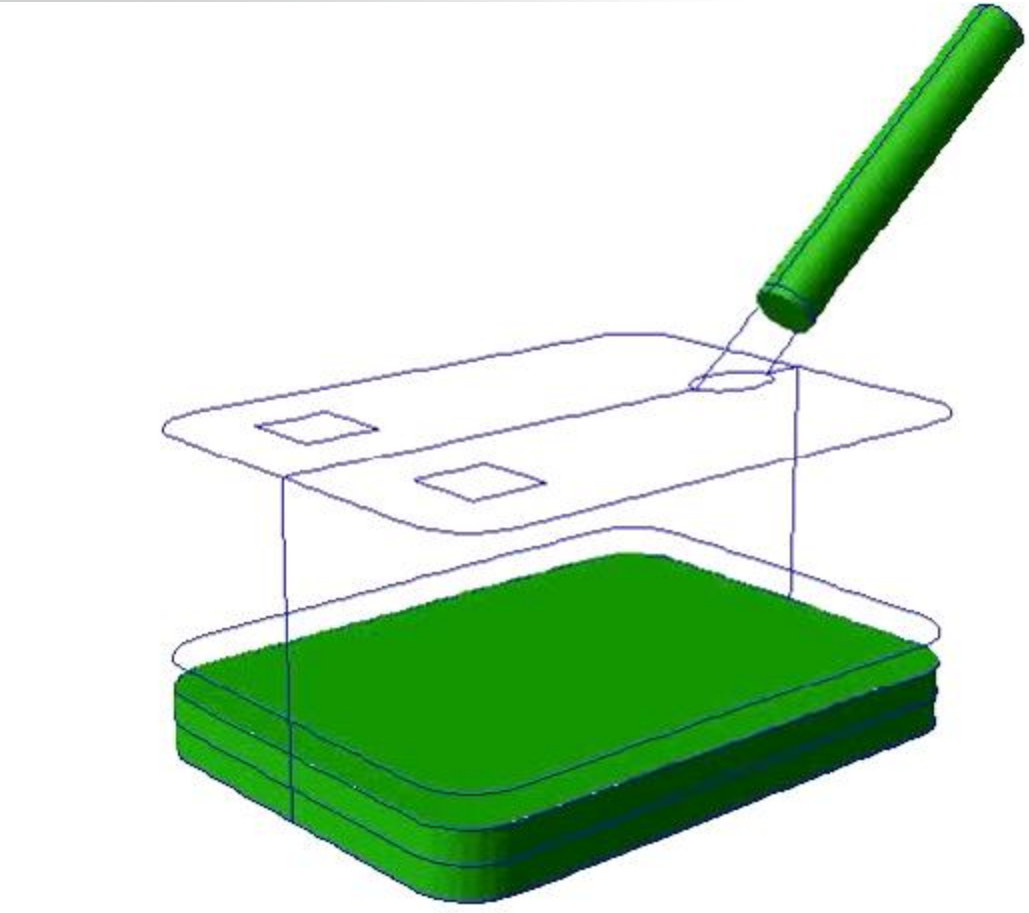
Tank Filling



- **Filling of a vessel**

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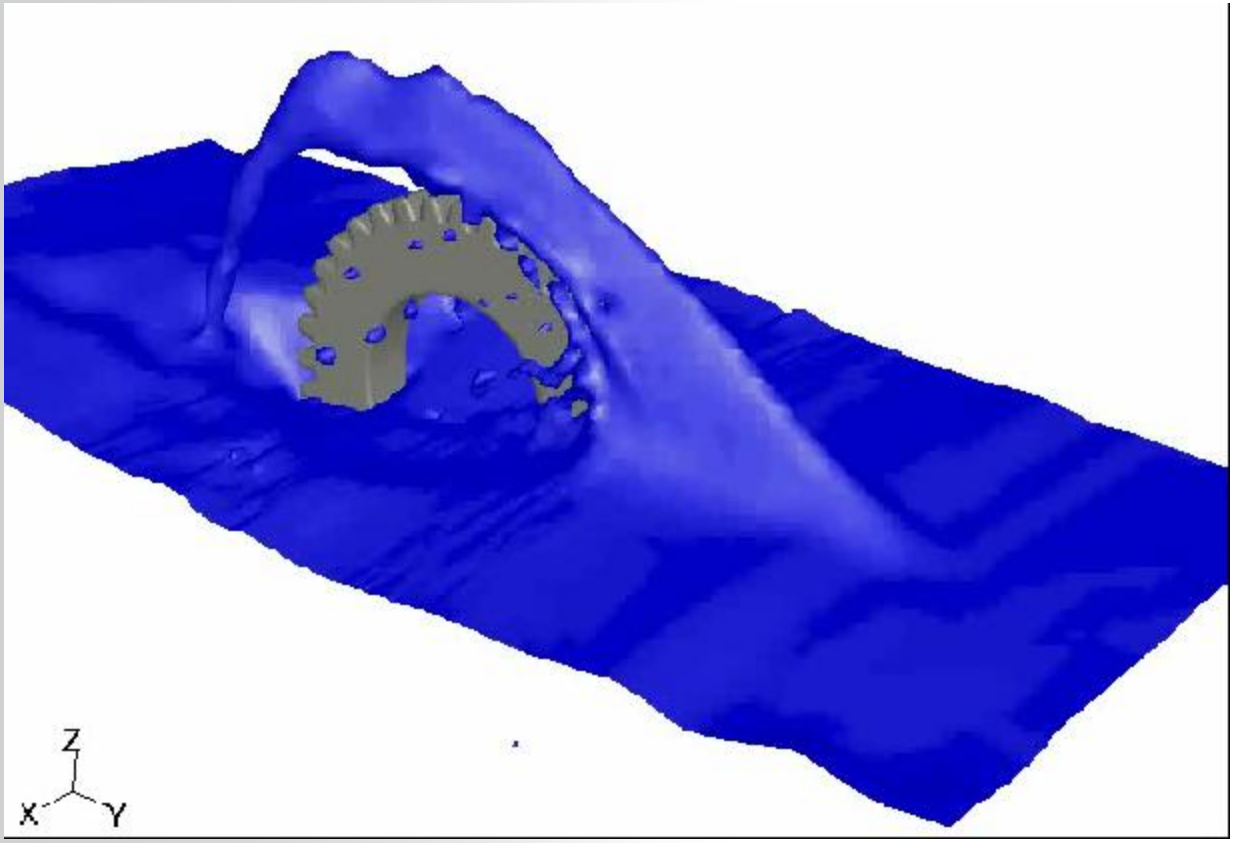
Free Surface Flow Around A Spinning Gear



- Sliding mesh model with VOF

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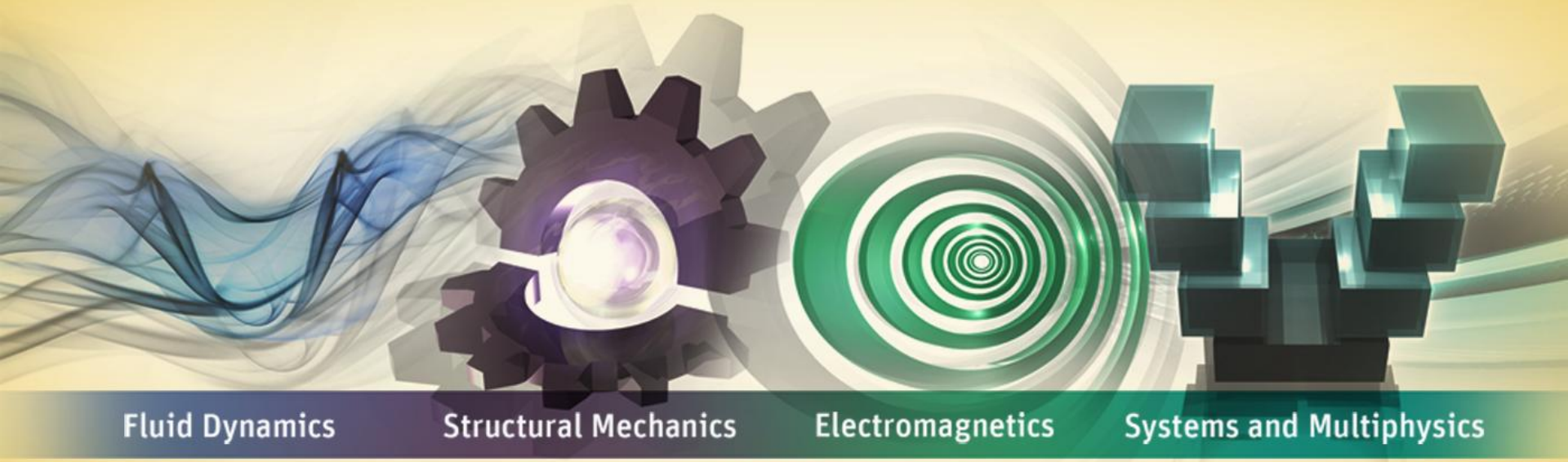
Volume Of Fluid Model In ANSYS CFX



Introduction

- There are cases where two continuous phases are separated by a distinct resolvable interface
  - Oil-water separators
  - Free surface flows
  - Break-up of droplets which are large relative to the grid scale

- There may or may not be slip between the phases:
  - Homogeneous: both phases are assumed to move with the same velocity (commonly assumed for free surface flows), less overhead since phases share all field variables except for volume fraction
  - Inhomogeneous: there may be slip between the two continuous phases - full overhead for multiple phases

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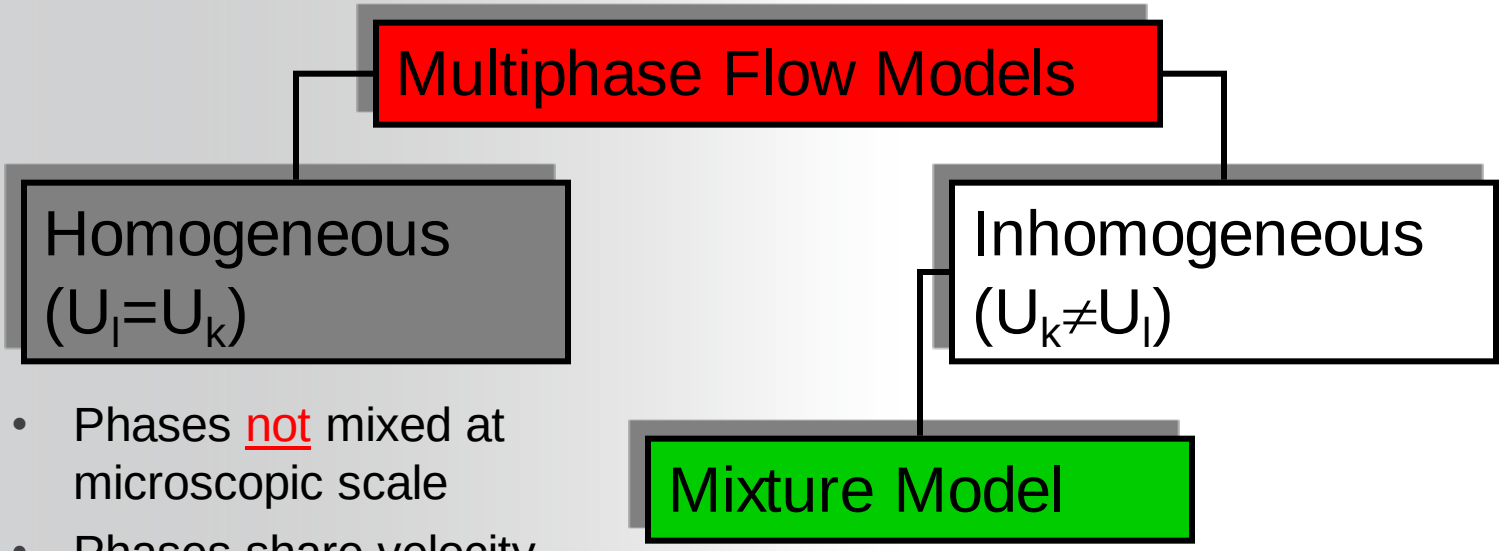
Modeling Strategies



- Phases not mixed at microscopic scale
- Phases share velocity field
- Free surface flows
- Disperse flows with high interfacial drag → small particles
- Drag prediction not required

- Complex interfacial boundaries
- Gas-liquid flows with flow regime transition

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Free Surface Flows

- Free surface flows
  - separated multiphase flow
  - fluids separated by distinct resolvable interface
  - examples: open channel flow, flow around ship hulls, water jet in air (Pelton wheel), tank filling, etc.
  - volume fractions are close to zero or unity except near the interface.

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Free Surface Applications

- Surface tension usually negligible
  - Mold filling
  - Metal solidification (melt interface)
  - Civil Hydraulics
  - Flows in tanks
- Surface tension usually important
  - Inkjets, dispensing
  - Silicon crystal growth
  - Coating (wire, dip, slide, extrusion)
  - Bio-microfluidics

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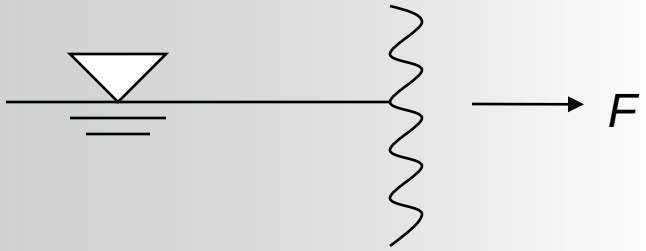
Surface Tension

- An attractive force at the free surface interface



$$\sigma = \frac{F}{L}$$

- Normal component
  - smooths regions of high curvature
  - induces pressure rise within droplet: $\Delta p = \sigma\kappa$
- Tangential component
  - moves fluid along interface toward region of high σ
  - often called Marangoni effect (σ decreases with temperature)

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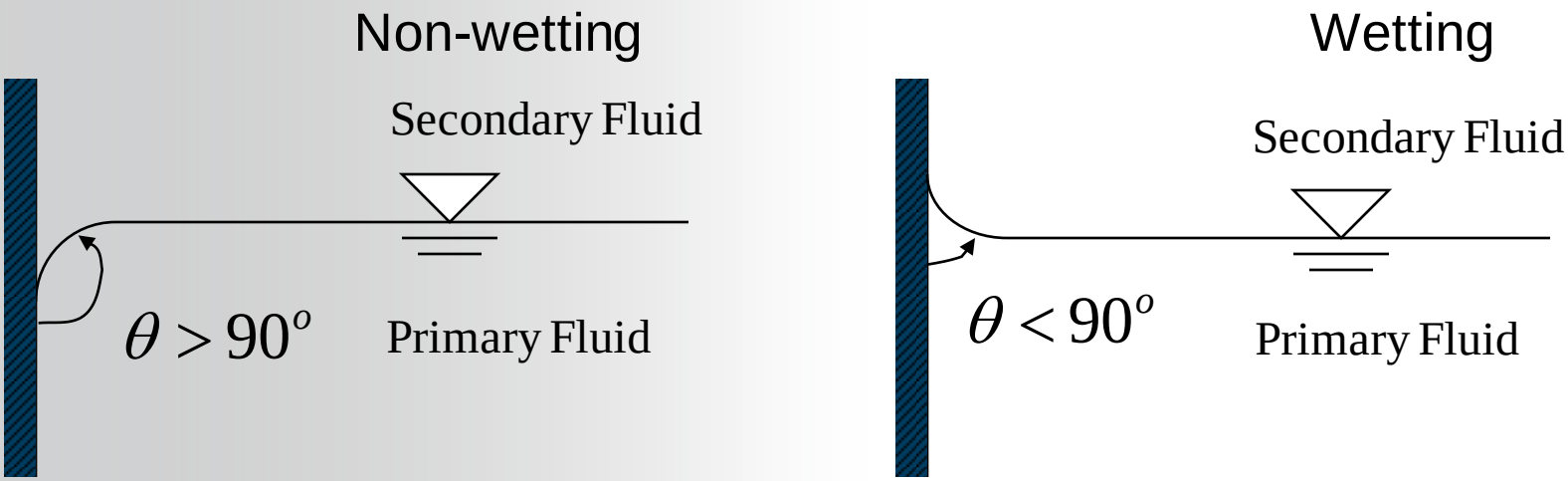
Wall Adhesion



- Wall adhesion is responsible for capillary rise in tubes

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Classifying Free Surface Flows

- In the absence of surface tension, use the Froude number to characterize the flow:

$$Fr = \frac{V}{\sqrt{gL}} = \frac{\text{convective speed}}{\text{wave speed}}$$

  - L=h (water depth) for shallow water flow
  - $L=\lambda/2\pi$ (wavelength) for sinusoidal wave train in deep water
  - for flow around ship hulls, there is not single wave velocity, but a Froude number can be defined for the ship geometry
- Analogies with Mach number
  - Flow can be subcritical, transcritical, or supercritical
  - For supercritical flow, the local velocity is greater than the surface wave speed, while subcritical flow has a velocity less than the wave speed.
  - A hydraulic jump occurs when the flow transitions from supercritical ($Fr > 1$) to subcritical ($Fr < 1$)

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Classifying Free Surface Flows

- If surface tension forces are important, different dimensionless groups may be useful:
  - Weber number (Re >> 1) - droplet formation

$$\mathrm{We} = \frac{\rho U^2 L}{\sigma} = \frac{\text{Inertial force}}{\text{Surface tension force}}$$

  - Capillary number (Re << 1) - coating flows

$$\mathrm{Ca} = \frac{\mu U}{\sigma} = \mathrm{Re}\,\mathrm{We} = \frac{\text{Viscous force}}{\text{Surface tension force}}$$

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Modeling Surface Tension

- Conceptually a surface force at interface

$$\vec{f}_s = -\sigma\kappa\hat{n} + \nabla_s\sigma$$

  - awkward to deal with interface topology

- Reformulate as a continuum force
  - Brackbill, Kothe, Zemach 1992

$$\vec{F}_s = \vec{f}_s\delta_s$$

$$\delta_s = |\nabla r|$$

$$\kappa = \nabla \cdot \hat{n}$$

$$\hat{n} = -\nabla r / |\nabla r|$$

  - wall contact angle specifies direction of normal at wall

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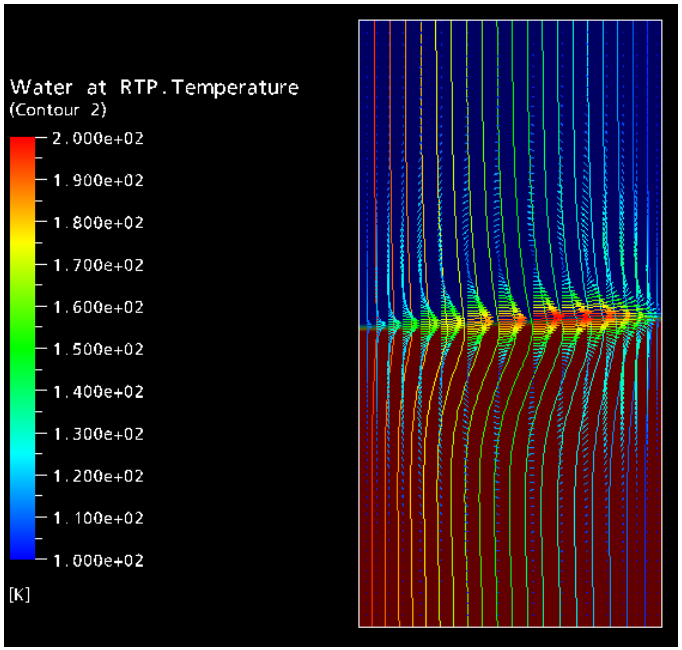
Surface Tension in ANSYS CFX

- Variable surface tension is implemented in ANSYS CFX (Marangoni flows)
  - in the example at right, a temperature gradient induces a surface tension gradient which gives rise to a tangential force at the interface



- VOF method
  - Interface tracked across fixed grid
  - Good for large deformations, robust
- For free surface flows, a compressive discretization scheme is used to sharpen the interface (smeared over 2-3 elements). This scheme is conservative.
- Pressure-velocity coupling (Rhie-Chow)
  - special treatment of buoyancy force to keep flow well-behaved at interface

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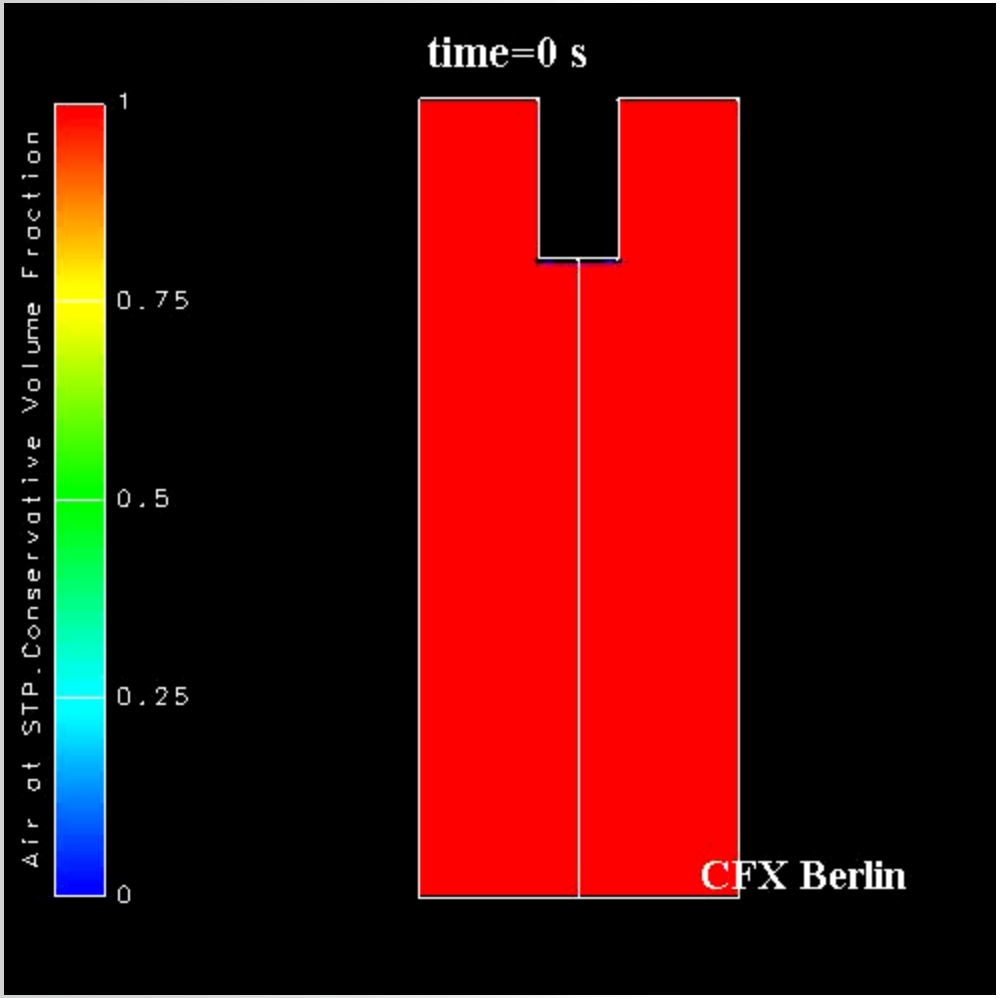
Surface Tension Example



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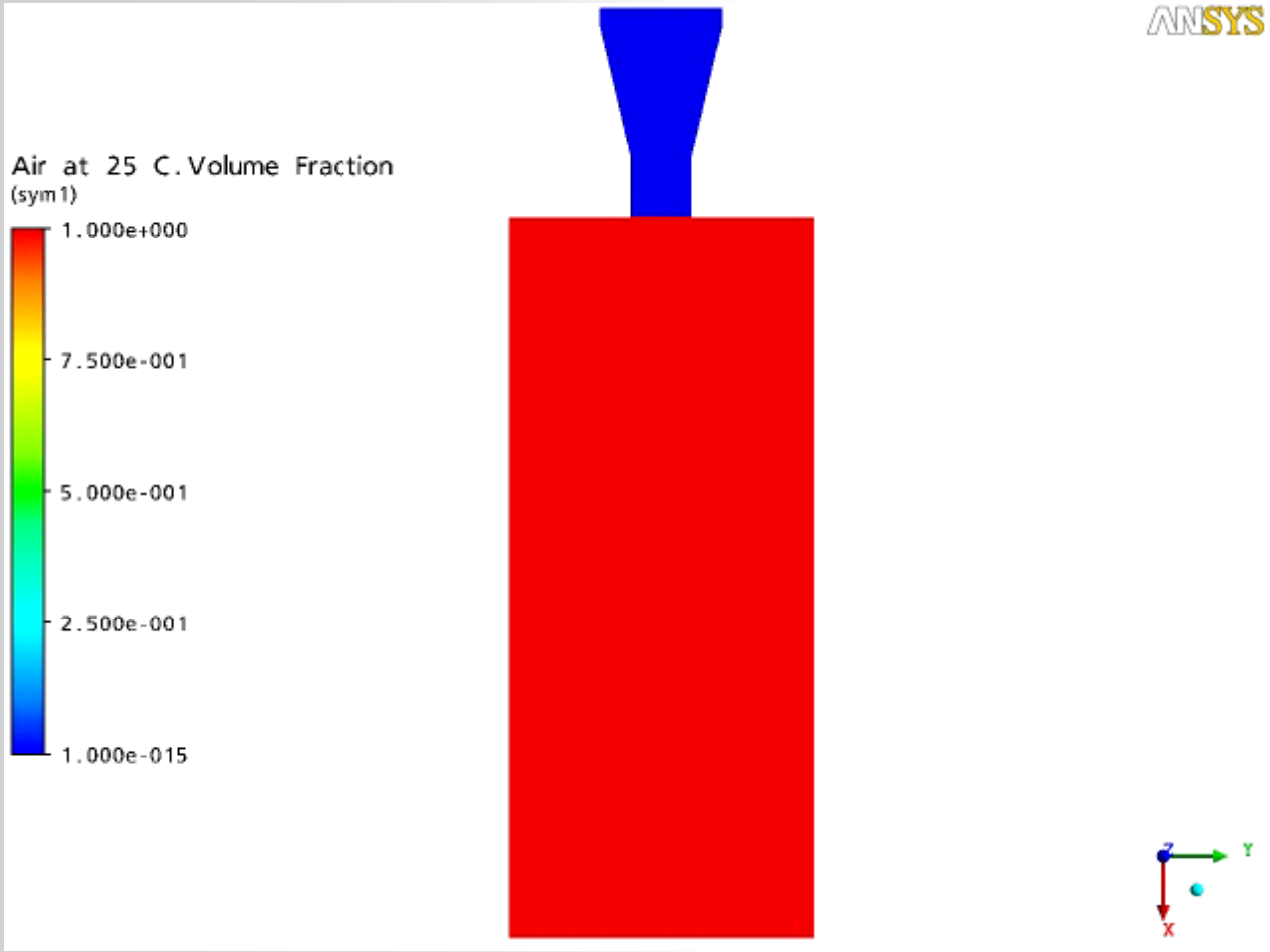
Inkjet Droplet Ejection

- Droplet ejected by pressure pulse prescribed to model piezoelectric actuator



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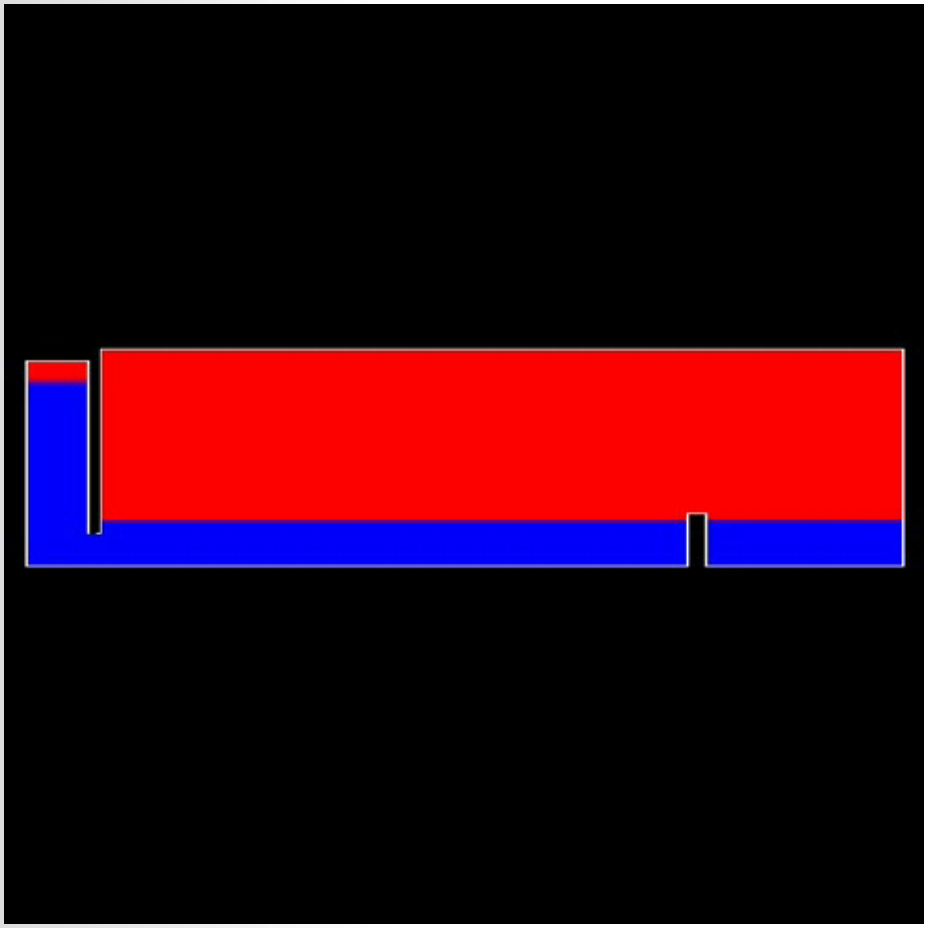
Free Surface Examples

- Maxwell's Experiment
- 2d transient problem



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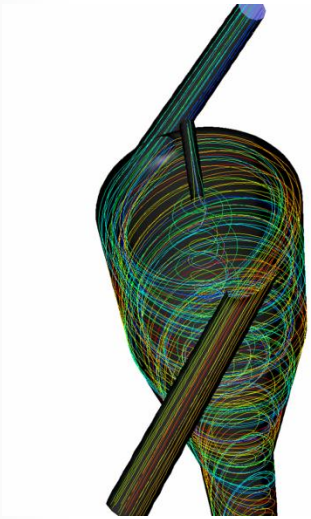
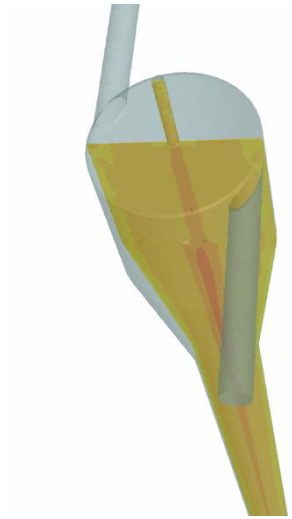
Summary – Multiphase Flow with ANSYS CFD

- **Dispersed-phase modeling in ANSYS CFD**
  - Capability of models
  - Examples

- **Volume of Fluid (VOF) modeling in ANSYS CFD**
  - FLUENT
  - CFX



Pathlines in deoiling hydrocyclone



Volume fracture of oil (mixture

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Questions?

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