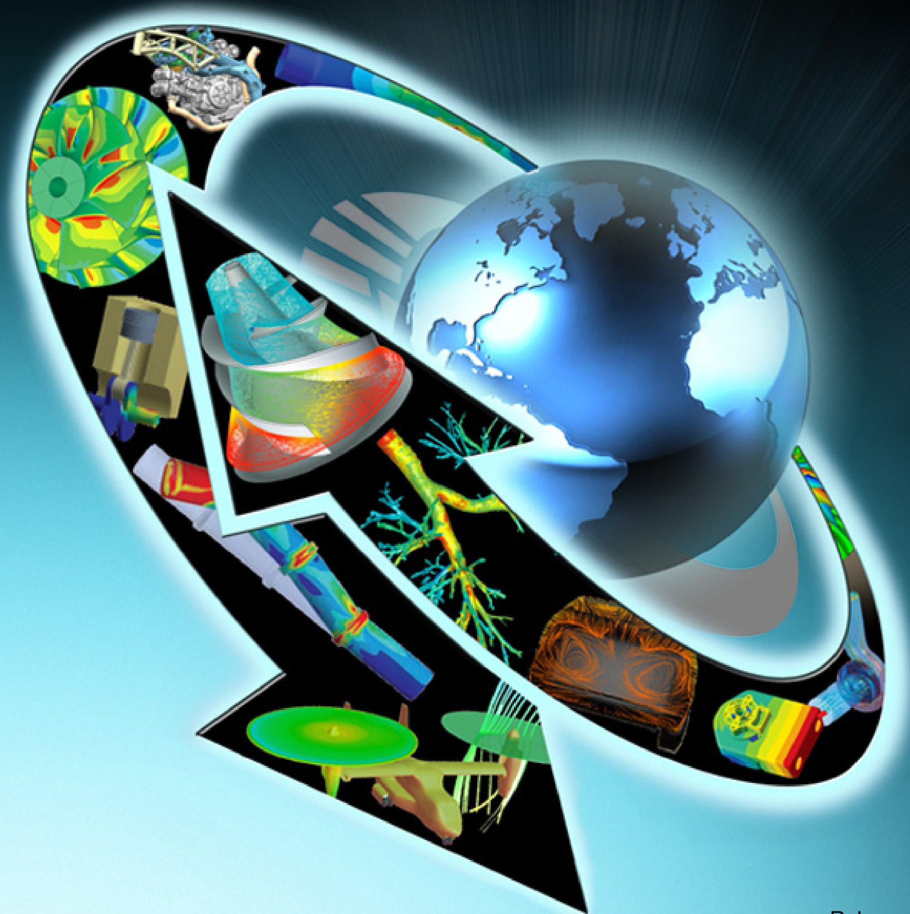
ANSYS®

Customer Training Material

Lecture 9

Advanced Physics



Introduction to ANSYS FLUENT

Release 13.0
December 2010

Outline

- **Multiphase Flow Modelling**
  - Discrete phase model
  - Eulerian model
  - Mixture model
  - Volume-of-Fluid (VOF) model

- **Reacting Flow Modelling**
  - Eddy dissipation model
  - Non-premixed, premixed and partially premixed combustion models
  - Detailed chemistry models
  - Pollutant formation
  - Surface reactions

- **Modelling Moving Parts**
  - Single and multiple reference frames
  - Mixing planes
  - Sliding meshes
  - Dynamic meshes
  - Six-degree-of-freedom solver

Multiphase Flows

Multiphase Flows - Introduction

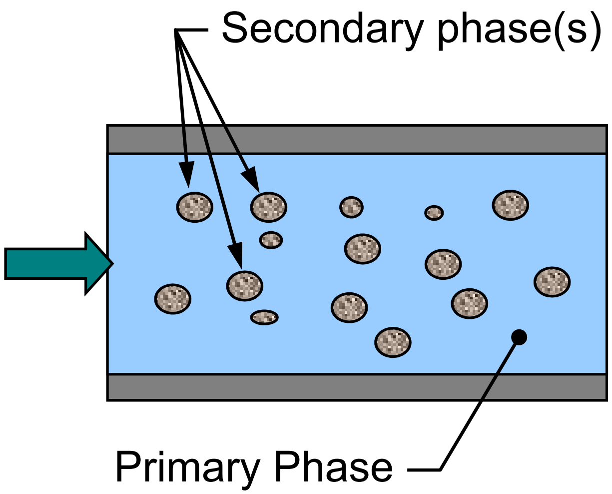
- In many flows, there is more than one fluid present in the domain
  - Different substances (eg oil & water, or methane & air)
  - Different phases of same substance (water & steam)

- The key issue is how these two fluids are **mixed**
  - If they are **mixed at a molecular level**, the problem is a **multi-species flow**.
  - A common example is where two gases are present (methane and air)
  - A diffusivity ('material property') is set for the mixture, and one extra transport equation is solved for the mass fraction of primary component.

  - If the mixing is more **macroscopic**, then it is a **multiphase flow**.
  - In such cases there is an identifiable boundary between the two phases
  - The user must therefore indicate to the solver how this boundary performs *maybe a free surface (VOF model), or a typical droplet size (mixture model)*

Multiphase Flows - Introduction

- The fluid system is defined by a primary and multiple secondary phases.
  - **One of the phases** is considered continuous (primary)
  - The others (secondary) are considered to be dispersed within the continuous phase.
  - *(Note that for free-surface flows, using the Volume of Fluid model, a distinct interface is defined between the phases and both could be considered continuous)*



Multiphase Flow Regimes

Gas/Liquid
Liquid/Liquid

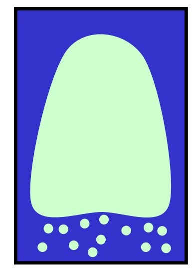
- **Bubbly flow** – Discrete gaseous bubbles in a continuous fluid, e.g. absorbers, evaporators, sparging devices.
- **Droplet flow** – Discrete fluid droplets in a continuous gas, e.g. atomizers, combustors
- **Slug flow** – Large bubbles in a continuous liquid
- **Stratified / free-surface flow** – Immiscible fluids separated by a clearly defined interface, e.g. free-surface flow

Gas / Solid

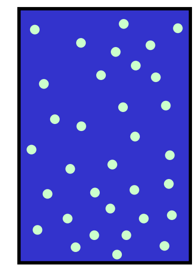
- **Particle-laden flow** – Discrete solid particles in a continuous fluid, e.g. cyclone separators, air classifiers, dust collectors, dust-laden environmental flows

Liquid / Solid

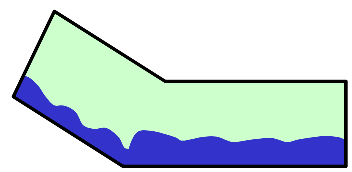
- **Fluidized beds** – Fluidized bed reactors
- **Slurry flow** – Particle flow in liquids, solids suspension, sedimentation, and hydro-transport



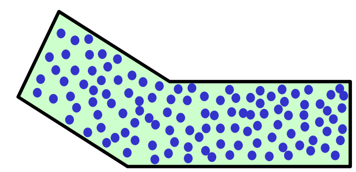
Slug Flow



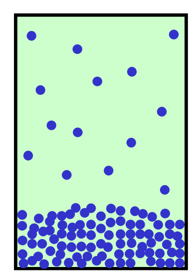
Bubbly, Droplet, or Particle-Laden Flow



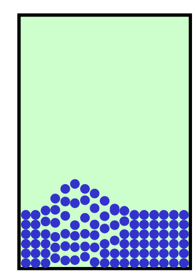
Stratified / Free-Surface Flow



Pneumatic Transport, Hydrotransport, or Slurry Flow



Sedimentation



Fluidized Bed

Multiphase Models Available in FLUENT

- FLUENT contains four distinct multiphase modeling approaches:
  - Discrete Phase Model (DPM)
  - Volume of Fluid Model (VOF)
  - Eulerian Model
  - Mixture Model

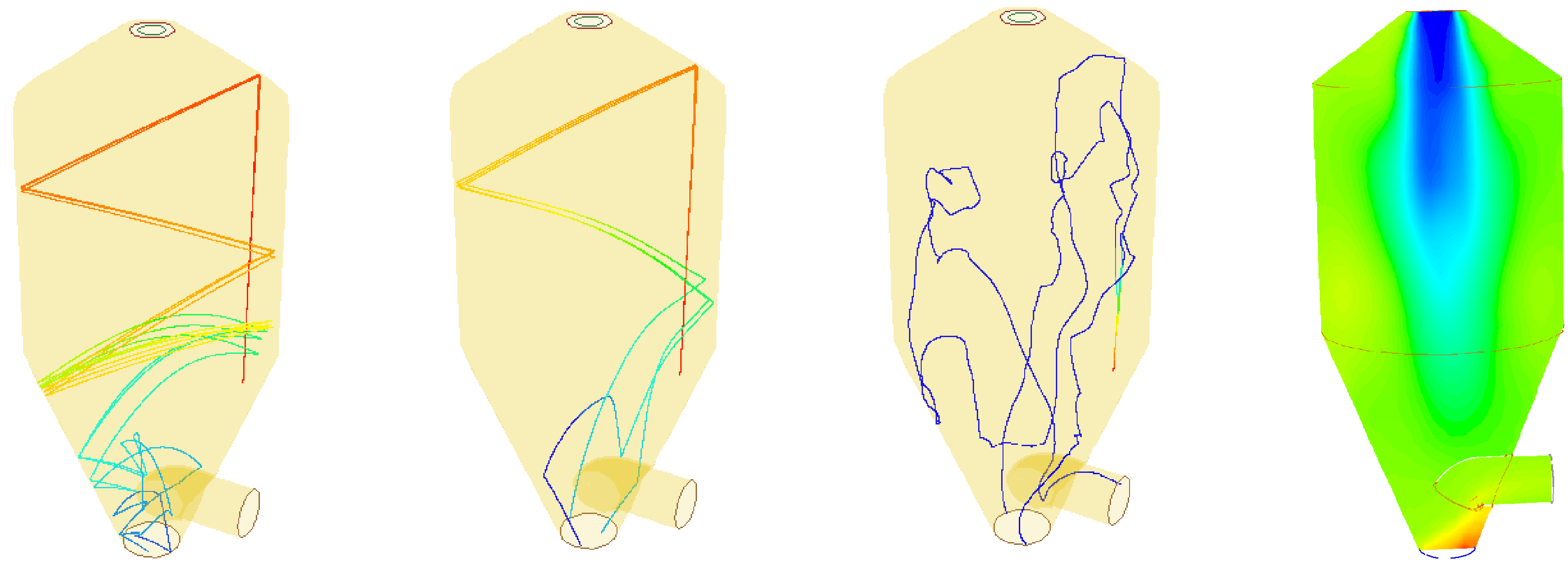
- It is important to select the most appropriate modelling approach when attempting to model a multiphase flow.
  - Depends on whether the flow is stratified or disperse – length scale of the interface between the phases dictates this.
  - Also the Stokes number (the ratio of the particle relaxation time to the characteristic time scale of the flow) should be considered.

$$\mathrm{St} = \frac{\text{Disperse phase time scale}}{\text{Continuous phase time scale}} = \frac{\tau_\mathrm{d}}{\tau_\mathrm{c}} \quad \text{where} \quad \tau_\mathrm{c} = \frac{D}{U} \quad \text{and} \quad \tau_\mathrm{d} = \frac{\rho_d d_d}{18\mu_c}$$

.

DPM Example – Spray Dryer

- Spray drying involves the transformation of a liquid spray into dry powder in a heated chamber. The flow, heat, and mass transfer are simulated using the DPM model in FLUENT.



Initial particle Diameter: 2 mm

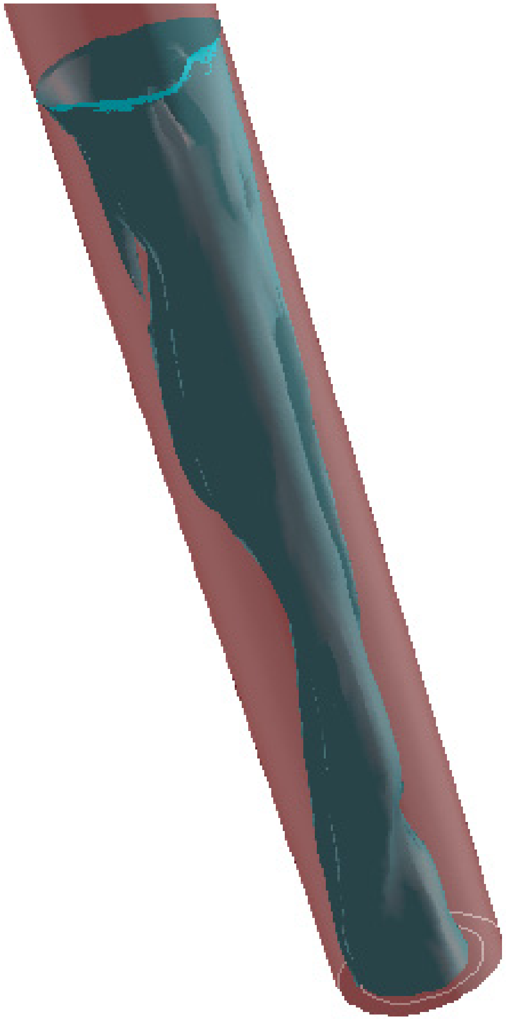
1.1 mm

0.2 mm

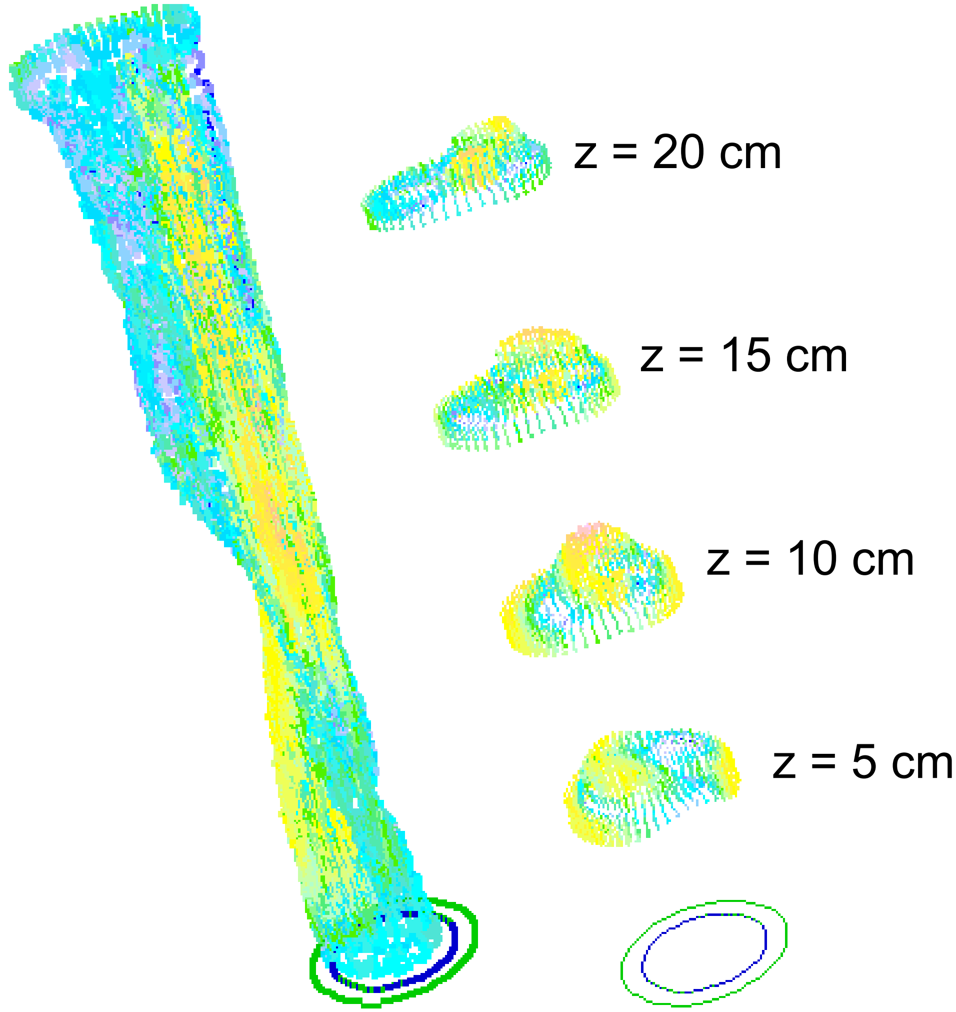
Contours of Evaporated Water

Stochastic Particle Trajectories for Different Initial Diameters

Eulerian Model Example – 3D Bubble Column



Isosurface of Gas Volume Fraction = 0.175



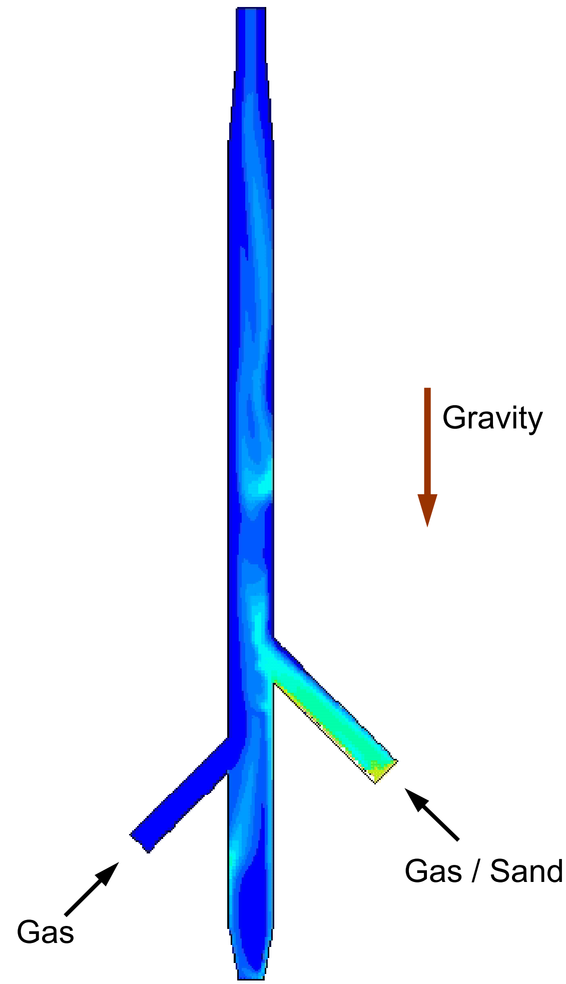
Liquid Velocity Vectors

The Granular Option in the Eulerian Model

- Granular flows occur when a high concentration of solid particles is present. This leads to high frequency of interparticle collisions.

- Particles are assumed to behave similarly to a dense cloud of colliding molecules. Molecular cloud theory is applied to the particle phase.

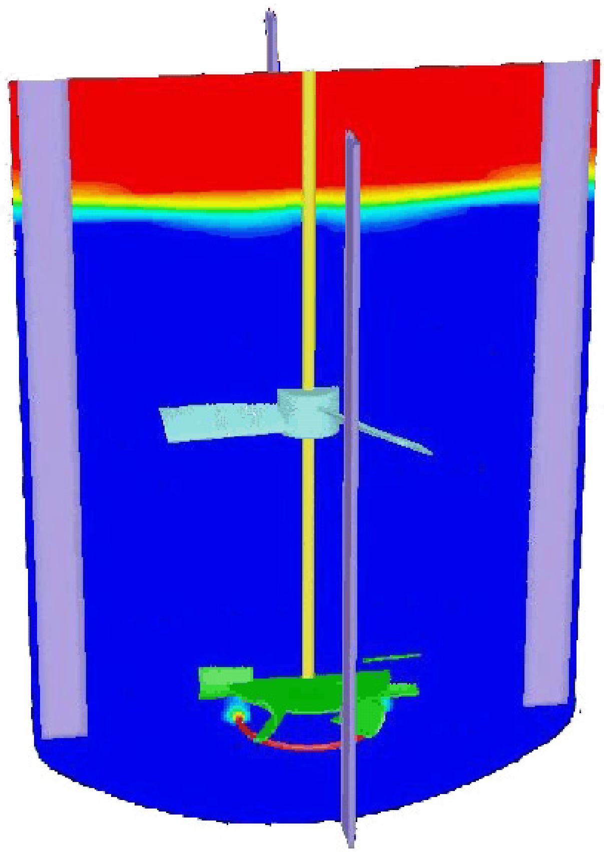
- Application of this theory leads to the appearance of additional stresses in the momentum equations for continuous and particle phases
  - These stresses (granular “viscosity”, “pressure” etc.) are determined by intensity of particle velocity fluctuations
  - Kinetic energy associated with particle velocity fluctuations is represented by a “pseudo-thermal” or granular temperature
  - Inelasticity of the granular phase is taken into account



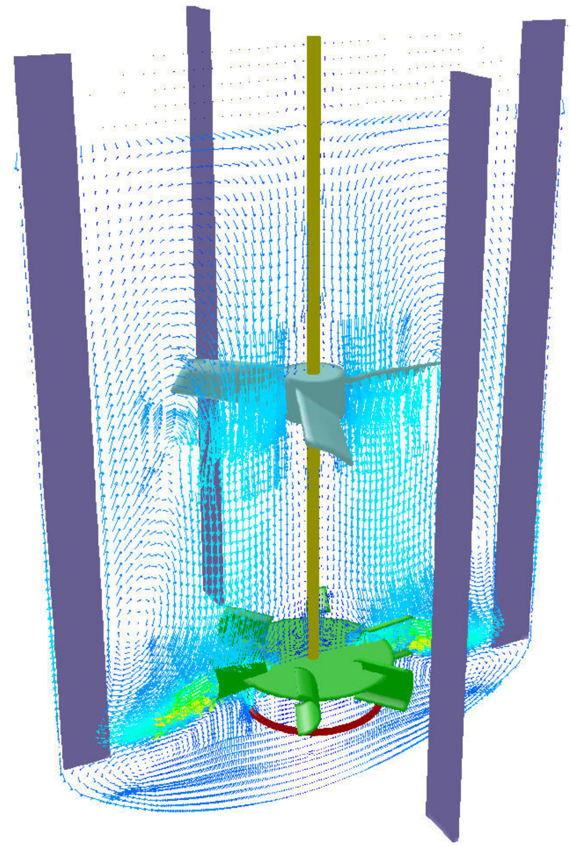
Contours of Solids Volume Fraction for High Velocity Gas/Sand Production

Mixture Model Example – Gas Sparging

- The sparging of nitrogen gas into a stirred tank is simulated by the mixture multiphase model. The rotating impeller is simulated using the multiple reference frame (MRF) approach.
- FLUENT simulation provided a good prediction on the gas-holdup of the agitation system.



Animation of Gas Volume Fraction Contours



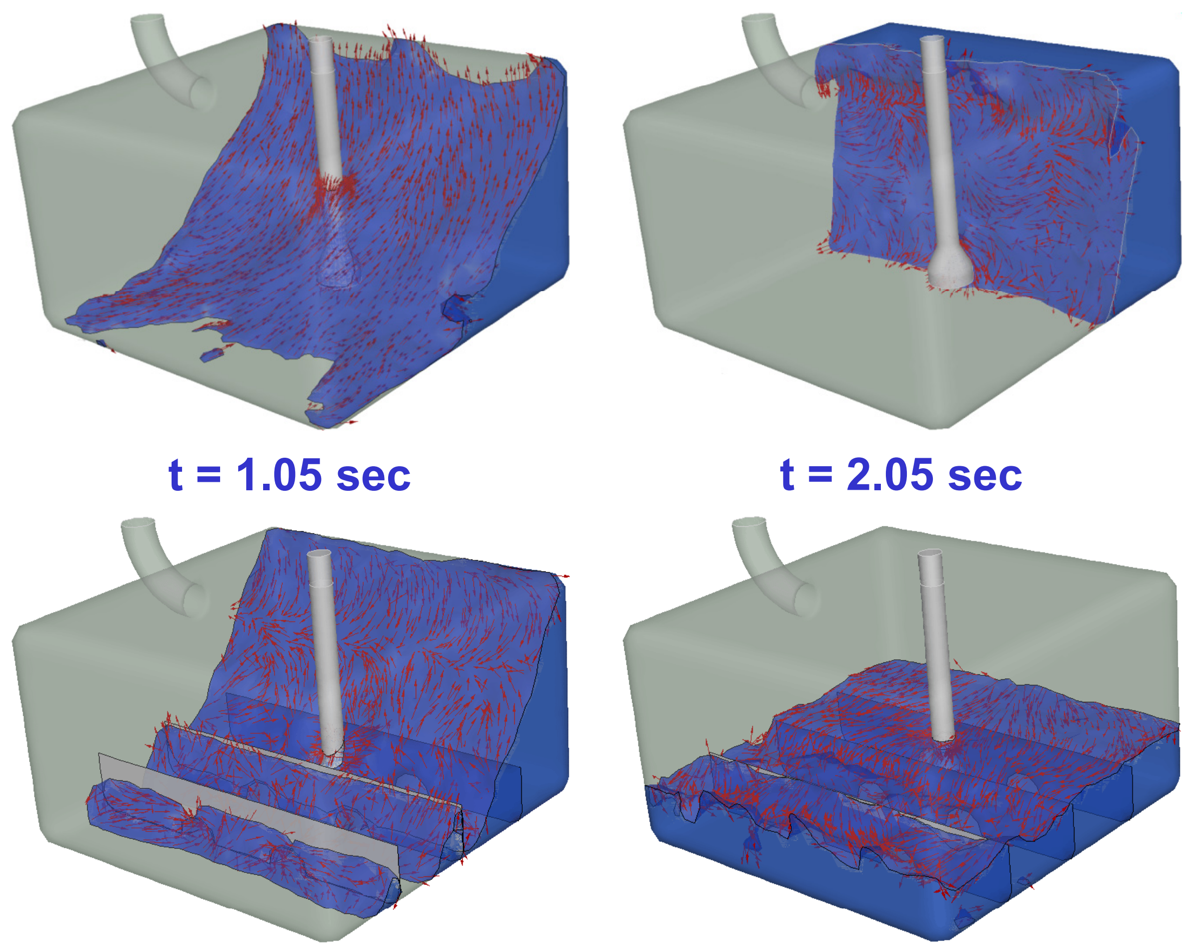
Water Velocity Vectors on a Central Plane at t = 15 sec.

VOF Example – Automobile Fuel Tank Sloshing

- Sloshing (free surface movement) of liquid in an automotive fuel tank under various accelerating conditions is simulated by the VOF model in FLUENT.

- Simulation shows that the tank with internal baffles will keep the fuel intake orifice fully submerged at all times compared to the tank with no baffles.

Fuel Tank Without Baffles



Fuel Tank With Baffles

Learning More

- Many more workshops are available.
- Look at www.fluentusers.com (same password as ANSYS portal)
  – Follow link to **ANSYS FLUENT > Advanced / Intermediate Tutorials**
    - Heat and Mass Transfer with the Mixture Model
    - Hydrodynamics of Bubble Column Reactors
    - Horizontal Film Boiling
    - Dam-Break Simulation Using FLUENT's Volume of Fluid Model
    - Using FLUENT's Erosion Model to Investigate Erosion in a 90 degree Elbow Bend
    - Using the Eulerian Multiphase Model with Species Transport
    - Modeling Flow and Heat Transfer in Packed Bed Reactor
    - Modeling Rapid Condensation of Steam in a 2D Laval Nozzle
    - Solving a 2D Box Falling into Water
    - Modeling Uniform Fluidization in 2D Fluidized Bed
    - Modeling Bubble Breakup and Coalescence in a Bubble Column Reactor
    - Spin Coating of a Rotating Circular Glass Substrate
    - Fuel Tank Sloshing
    - Continuous Steel Casting of a Round Billet
    - Modeling the Effect of Sedimentation Concentration using a UDF
    - Modeling Nucleate Boiling using FLUENT
- *We also strongly recommend attending our Advanced Multiphase Training*

Reacting Flows

Reacting Flows Introduction

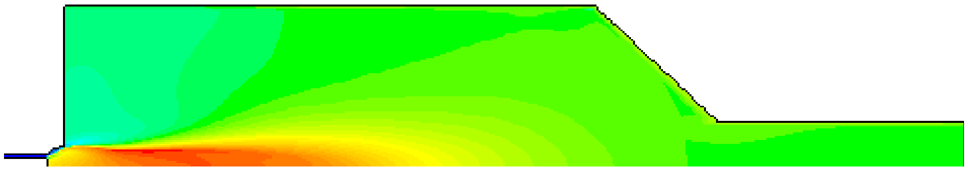
- So far we have assumed that whatever materials are entering the domain are the same as those leaving the domain.

- However in some cases the materials entering will react with each other to form new products (CO_2 , H_2O , NO_x etc)

- By defining the reaction chemistry and kinetics, FLUENT can compute the chemical reaction.
  - Within the flow domain, we have already seen how the solver can compute the species concentration and temperature.
  - This can then be combined with knowledge of the reaction to form new species in the model, with a corresponding transfer of energy.

Applications of Reacting Flow Systems

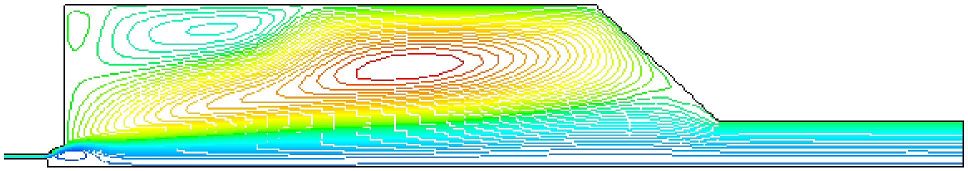
- FLUENT contains models which are applicable to a wide range of homogeneous and heterogeneous reacting flows
  - Furnaces
  - Boilers
  - Process heaters
  - Gas turbines
  - Rocket engines
  - IC engine
  - CVD, catalytic reactions



Temperature in a Gas Furnace

CO_2 Mass Fraction

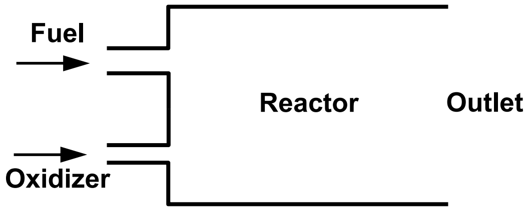
- Predictions of
  - Flow field and mixing characteristics
  - Temperature field
  - Species concentrations
  - Particulates and pollutants



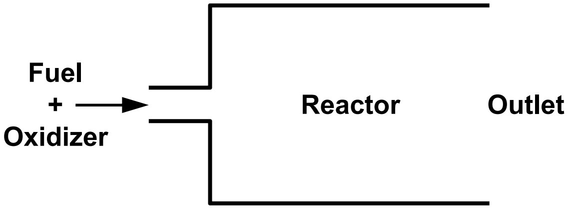
Stream Function

Background

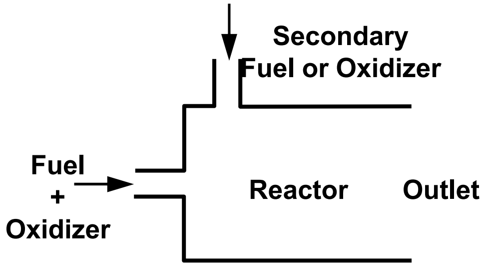
- Modeling Chemical Kinetics in Combustion
  - Fast Chemistry
    - Global chemical reaction mechanisms (Finite Rate / Eddy Dissipation)
    - Equilibrium/flamelet model (Mixture fraction)
  - Finite rate chemistry



- Flow configuration
  - Non-premixed reaction systems
    - Can be simplified to a mixing problem



  - Premixed reaction systems
    - Cold reactants propagate into hot products.



  - Partially premixed systems
    - Reacting system with both non-premixed and premixed inlet streams.

Overview of Reacting Flow Models in FLUENT

FLOW CONFIGURATION

CHEMISTRY

<table>
<tr><th></th><th>Premixed</th><th>Non-Premixed</th><th>Partially Premixed</th></tr>
<tr><td rowspan="2">Fast Chemistry</td><td colspan="3">Eddy Dissipation Model
(Species Transport)</td></tr>
<tr><td>Premixed Combustion Model
Reaction Progress Variable*</td><td>Non-Premixed Equilibrium Model
Mixture Fraction</td><td>Partially Premixed Model
Reaction Progress Variable
+
Mixture Fraction</td></tr>
<tr><td rowspan="4">Finite-Rate Chemistry</td><td></td><td colspan="2">Laminar Flamelet Model</td></tr>
<tr><td colspan="3">Laminar Finite-Rate Model</td></tr>
<tr><td colspan="3">Eddy-Dissipation Concept (EDC) Model</td></tr>
<tr><td colspan="3">Composition PDF Transport Model</td></tr>
</table>

***Rate classification not truly applicable since species mass fraction is not determined.**

Pollutant Formation Models

- **NOx formation models** (predict qualitative trends of NOx formation).
  - FLUENT contains three mechanisms for calculating NOx production.
    - Thermal NOx
    - Prompt NOx
    - Fuel NOx
  - NOx reburning model
  - Selective Non-Catalytic Reduction (SNCR) model
    - Ammonia and urea injection

- **Soot formation models**
  - Moos-Brookes model
  - One step and two steps model
  - Soot affects the radiation absorption (Enable the Soot-Radiation option in the Soot panel)

- **SOx formation models**
  - Additional equations for SO2, H2S, and, optionally, SO3 are solved.
  - In general, SOx prediction is performed as a post-process.

Discrete Phase Model (DPM)

- The reactions need not be restricted to the fluids in the model, the Discrete Phase model can also be used to simulate reacting particles – for example the combustion of pulverised coal particulates.

- Numerous submodels are available.
  - Heating/cooling of the discrete phase
  - Vaporization and boiling of liquid droplets
  - Volatile evolution and char combustion for combusting particles
  - Droplet breakup and coalescence using spray models
  - Erosion/Accretion

- Numerous applications
  - Particle separation and classification, spray drying, aerosol dispersion, bubble sparging of liquids, liquid fuel and coal combustion.

Surface Reactions

- Some reactions occur just on the wall surface (for example, in a vehicle's catalytic converter).
- Chemical species deposited onto surfaces are treated as distinct from the same chemical species in the gas.
- Site balance equation is solved for every surface-adsorbed (or "site") species.
  - Detailed surface reaction mechanisms can be considered (any number of reaction steps and any number of gas-phases or/and site species).
  - Surface chemistry mechanism in Surface CHEMKIN format can be imported into FLUENT.
  - Surface reaction can occur at a wall or in porous media.
  - Different surface reaction mechanisms can be specified on different surfaces.
- Application examples
  - Catalytic reactions
  - CVD

Learning More

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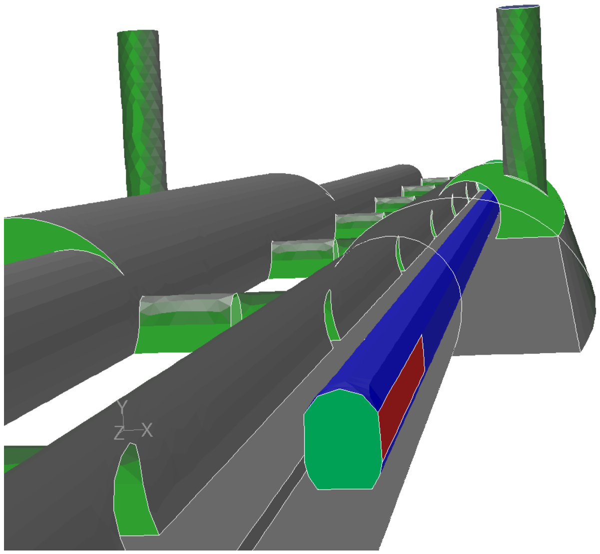
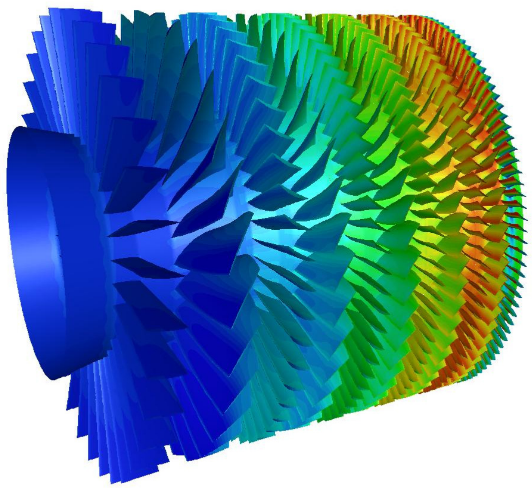
- Look at www.fluentusers.com (same password as ANSYS portal)
  - Follow link to **ANSYS FLUENT > Advanced / Intermediate Tutorials**
    - Coal Combustion with Eddy Break Up (EBU) Model
    - Modeling Liquid Reactions in a CIJR using the Unsteady Laminar Flamelet Model
    - Simulation of a Piloted Jet Flame using Unsteady Laminar Flamelet Model
    - 2D Simulation of a 300 KW BERL Combustor Using the Magnussen Model
    - Premixed Flow in a Conical Chamber using the Finite-Rate Chemistry Model
    - PDF Transport Simulation of a Piloted Jet Diffusion Flame
    - Liquid Fuel Combustion
    - 3D Simulation of 300 kW BERL Combustor Using the Laminar Flamelet Model
    - NOx Modeling with the SNCR Model Using Urea Injection
    - Modeling Liquid Reactions in a CIJR using the Unsteady Laminar Flamelet Model
    - Simulation of a Piloted Jet Flame using Unsteady Laminar Flamelet Model
    - EDC Simulation of a Piloted Jet Diffusion Flame
    - Premixed Combustion in a Conical Chamber using the Zimont Model
    - Modeling Surface Reaction in a Single Circular Channel
    - Multiple Char Reactions
    - Partially Premixed Combustion in a Coaxial Combustor
    - Modeling Evaporation of Liquid Droplets in a Circular Channel
- *We also strongly recommend attending our Advanced Combustion Course*

Modelling Moving Parts

Introduction

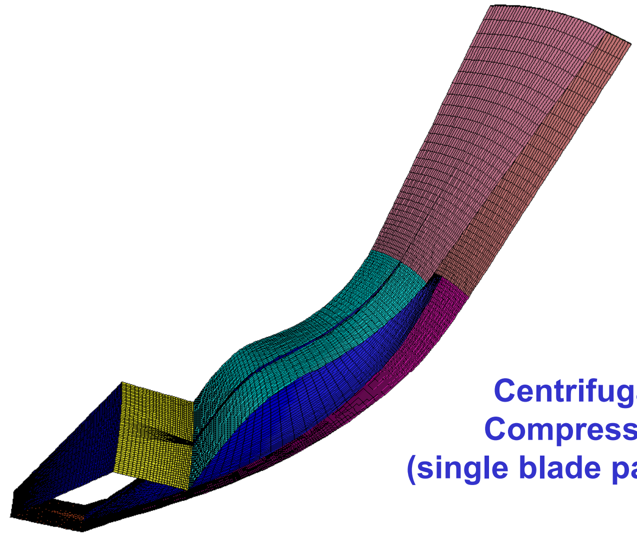
- Many flow problems involve domains which exhibit forms of motion.
- Two types of motion are possible – translational and rotational.
- There are two modeling approaches for moving domains:
  - Moving Reference Frames
    - Frame of reference is attached to the moving domain.
    - Governing equations are modified to account for moving frame.
  - Moving / Deforming Domains
    - Domain position and shape are tracked with respect to a stationary reference frame.
    - Solutions are inherently transient.





Single Reference Frame (SRF) Modeling

- **SRF** attaches a reference frame to a single moving domain.
  - All fluid motion is defined with respect to the moving frame.
  - Rotating frames introduce additional accelerations to the equations of fluid mechanics, which are added by Fluent when you activate a moving reference frame.
- Why use a moving reference frame?
  - Flow field which is transient when viewed in a stationary frame can become steady when viewed in a moving frame.
  - Advantages
    - Steady state solution*
    - Simpler BCs
    - Faster turn-around time
    - Easier to post-process and analyze



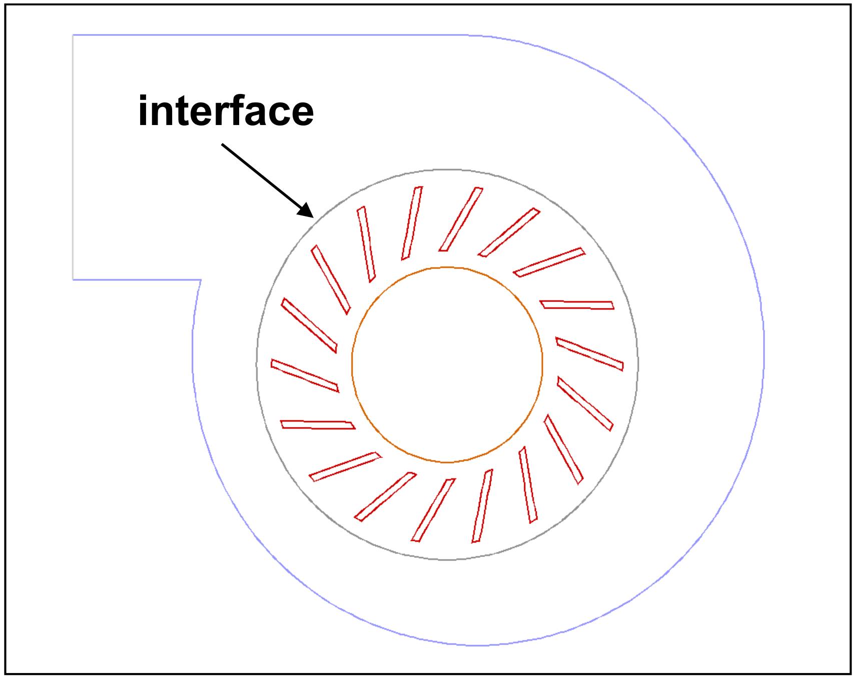
* NOTE: You may still have unsteadiness in the rotating frame due to turbulence, circumferentially non-uniform variations in flow, separation, etc. example: vortex shedding from fan blade trailing edge

Multiple Reference Frame (MRF) Modeling

- Many moving zone problems involve stationary components which cannot be described by surfaces of revolution (SRF not valid).
- Systems like these can be solved by dividing the domain into **multiple fluid zones** – some zones will be rotating, others stationary.
- The multiple zones communicate across one or more **interfaces** *(these may or may not be non-conformal)*
- The way in which the interface is treated leads to one of following approaches for multiple zone models:
  - Multiple Reference Frame Model (MRF)
  - Mixing Plane Model (MPM)
  - Sliding mesh model (SMM)

Steady State (Approximate)

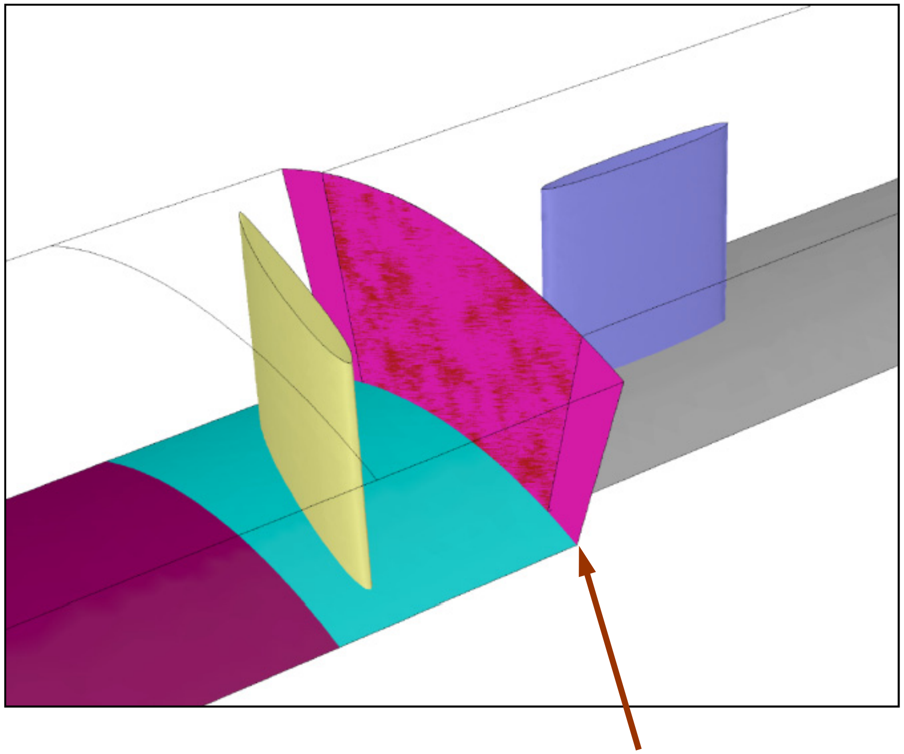
Transient (Best Accuracy)



Multiple Component (blower wheel + casing)

The Mixing Plane Model (MPM)

- The **MPM** is a technique which permits steady-state solutions for multistage axial and centrifugal turbomachines.
- Domain is comprised of multiple zones
- Each zone is “self contained” with a inlet, outlet, *wall*, periodic BCs
- Steady-state SRF solutions are obtained in each domain, with the domains linked by passing boundary conditions.
- The BC “links” between the domains are called mixing planes.
- BCs are passed as **circumferentially averaged profiles** of flow variables, which are updated at each iteration.



ADVANTAGE of MPM: Requires only a single blade passage per blade row regardless of the number of blades.

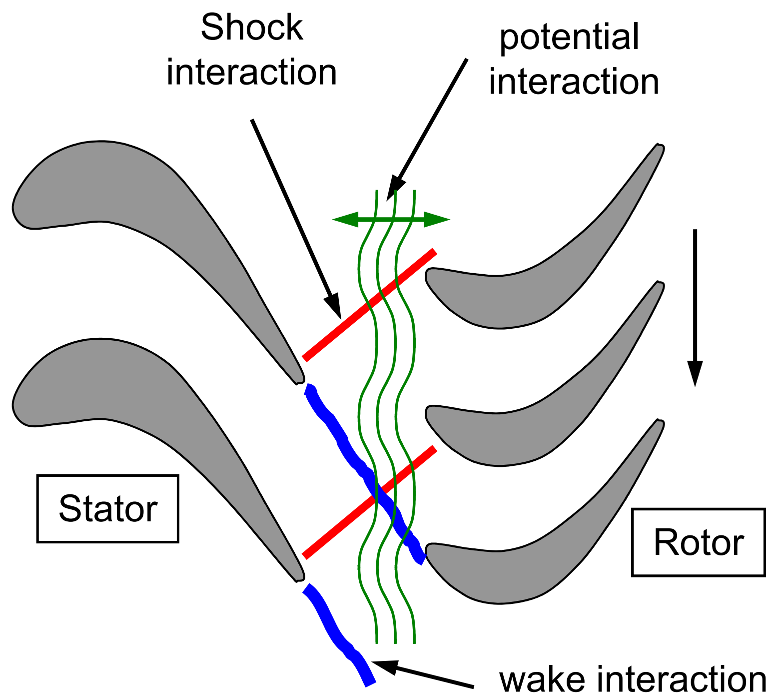
The Sliding Mesh Model (SMM)

- Although MRF and MPM are good for indicating the overall behaviour arising from the motion, they will not capture the transient detail as one object (and its wake) passes another.

- So, for example, the image shows where there may be a transient issue with shock interaction between rotor and stator.

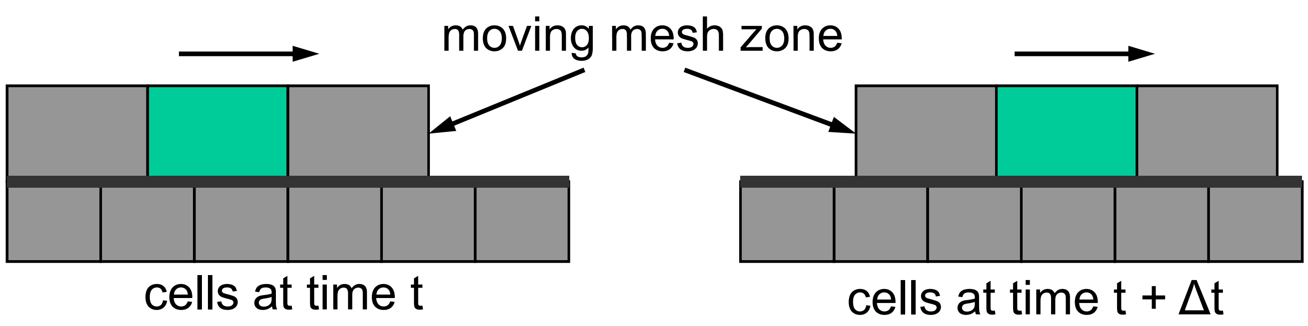
- If transient interaction can not be neglected, we can employ the Sliding Mesh model (SMM) to account for the relative motion between the stationary and rotating components.

- **Sliding Mesh** cases are always run in a transient manner, and one region of grid cells is moved (rotated or translated) each time step.



How the Sliding Mesh Model Works

- Like the MRF model, the domain is divided into moving and stationary zones, separated by **non-conformal interfaces**.

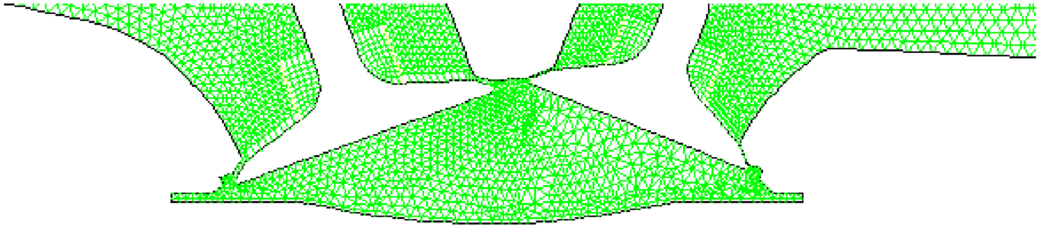


- Governing equations have a new moving mesh form, and are solved in the **stationary reference frame for absolute quantities** (see Appendix for more details).
  - Moving reference frame formulation is NOT used here (i.e. no additional accelerations acting as sources terms in the momentum equations).
  - Equations are a special case of the general moving/deforming mesh formulation.

The Dynamic Mesh (DMM) Model

- FLUENT can take mesh motion one step further, and modify the mesh in the solver at every time step so as to resolve larger motions (that would be impossible to account for with sliding meshes or MRF

- Examples:
  - Automotive piston moving inside a cylinder
  - Positive displacement pumps
  - A flap moving on an airplane wing
  - A valve opening and closing
  - An artery expanding and contracting



Dynamic Mesh (DM) Methods

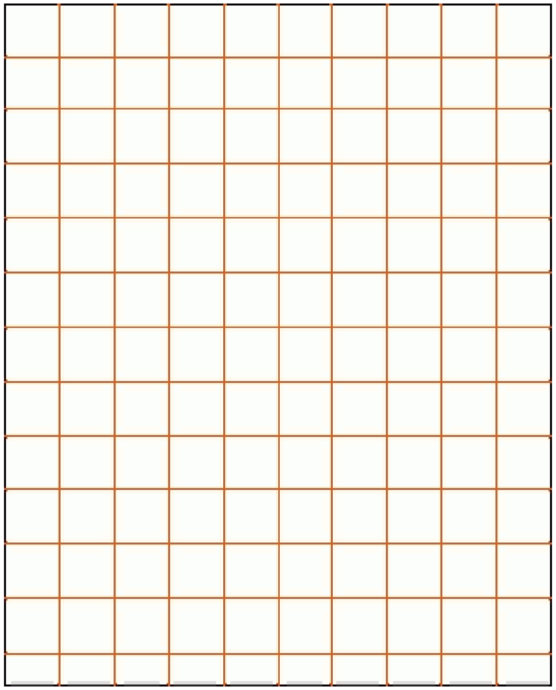
- Internal node positions are automatically calculated based on user specified boundary/object motion, cell type, and meshing schemes

- Basic Schemes
  - **Smoothing** (Spring analogy)
  - **Local remeshing**
  - **Layering**

- Other Methods
  - 2.5 D
  - User defined mesh motion
  - In-cylinder motion (RPM, stroke length, crank angle, …)
  - Prescribed motion via profiles or UDF
  - Coupled motion based on hydrodynamic forces from the flow solution, via FLUENT's six-degree-of-freedom (6DOF) solver.

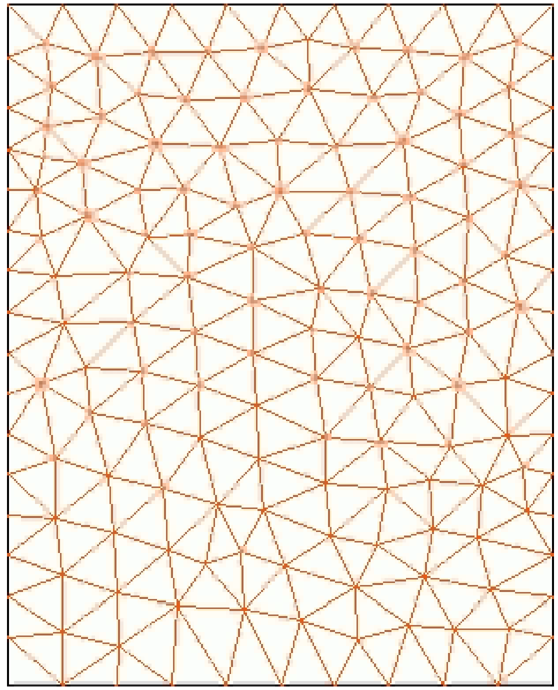
Dynamic Mesh Methods

Customer Training Material



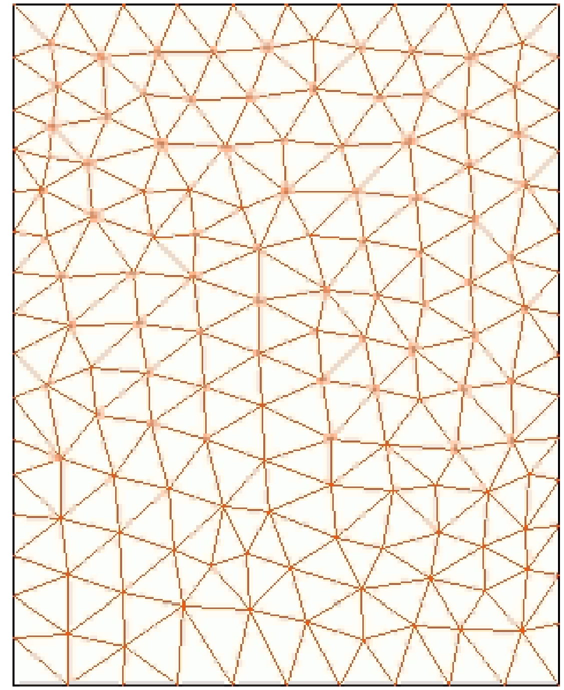
Layering

Layers of cells are generated and collapsed as they are overrun by the moving boundary. Layering is appropriate for quad/hex/prism meshes with linear or rotational motion and can tolerate small or large boundary deflections.



Local Remeshing

In local remeshing, as cells become skewed due to moving boundaries, cells are collapsed and the skewed region is remeshed. Local remeshing is appropriate for tri/tet meshes with large range of boundary motion.



Spring Analogy

Spring analogy is useful when there are small boundary deformations. The connectivity and cell count is unchanged during motion. Spring analogy is appropriate for tri/tet meshes with small deformations.

Summary

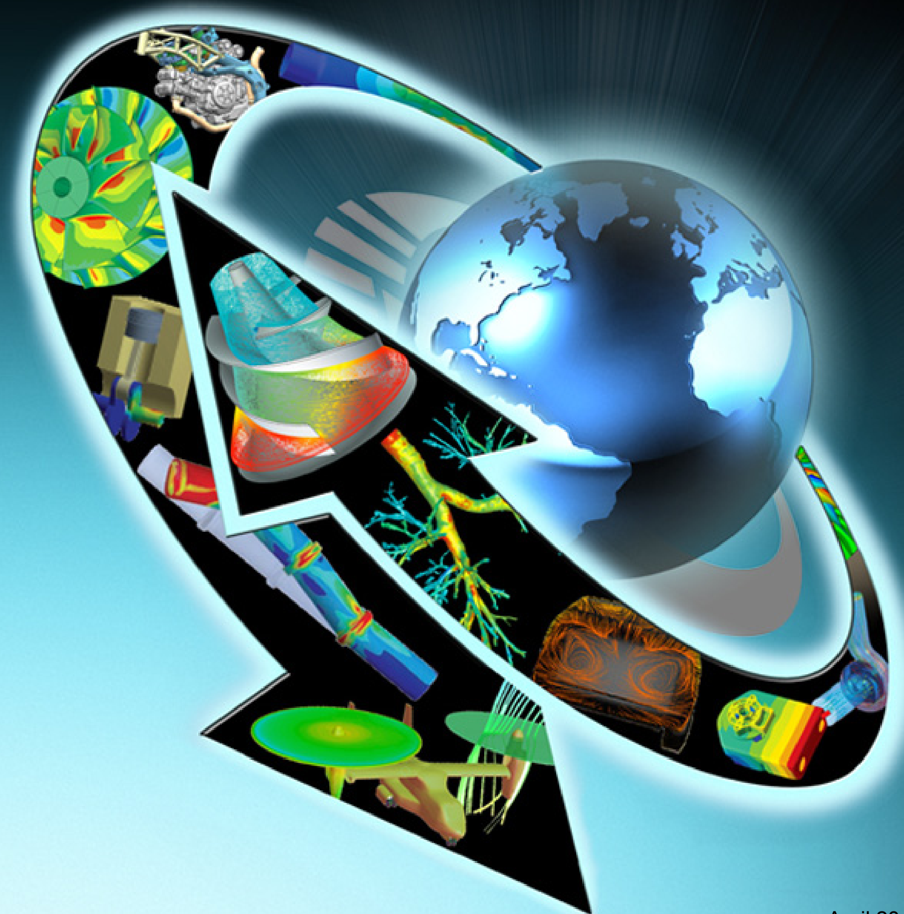
- Five different approaches may be used to model flows over moving parts.
  - Single (Rotating) Reference Frame Model
  - Multiple Reference Frame Model
  - Mixing Plane Model
  - Sliding Mesh Model
  - Dynamic Mesh Model
- First three methods are primarily steady-state approaches while sliding mesh and dynamic mesh are inherently transient.
- Enabling these models, involves in part, changing the stationary fluid zones to either Moving Reference Frame or Moving Mesh.
- Most physical models are compatible with moving reference frames or moving meshes (e.g. multiphase, combustion, heat transfer, etc.)

Learning More

- Many more workshops are available.
- Look at www.fluentusers.com (same password as ANSYS portal)
  - Follow link to **ANSYS FLUENT > Advanced / Intermediate Tutorials**
    - 2D Adiabatic Compression (Remeshing and Spring Smoothing)
    - 2D Adiabatic Compression (Layering)
    - 3D Adiabatic Compression (Layering, Remeshing, and Spring Smoothing)
    - Solving a 2D Box Falling into Water
    - Simulating a 2D Check Valve using FLUENT's DMM and Spring Smoothing
    - Submarine Docking Simulation Using MDM Model
    - Using a UDF to Control the Dynamic Mesh of a Flexible Oscillating Membrane
    - Solving a 2D Vibromixer Problem Using the Dynamic Mesh Model
    - Store Separation from a 3D Delta Wing
    - Projectile Moving Inside a Barrel
- *We also strongly recommend attending our Dynamic Mesh Training*

Appendix 1

Multiphase Flow Modeling

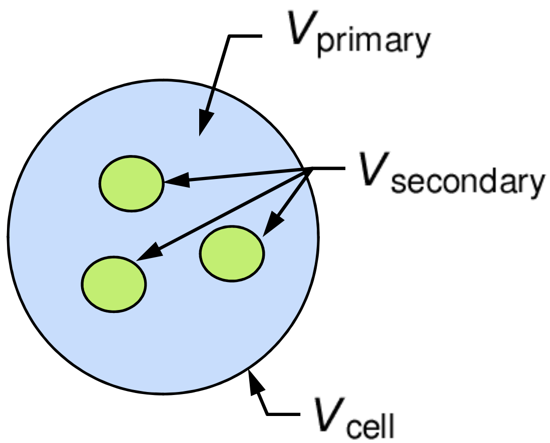


Volume and Particulate Loading

- Volume loading – dilute vs. dense
  - Refers to the volume fraction of secondary phase(s)

$$\text{Volume Fraction} = \alpha = \frac{\text{Volume of Phase in Cell/Domain}}{\text{Volume of Cell/Domain}}$$

  - For dilute loading (less than around 10%), the average inter-particle distance is around twice the particle diameter. Thus, interactions among particles can be neglected.



- Particulate loading – ratio of dispersed and continuous phase inertia.

$$\frac{\alpha_d \rho_d}{\alpha_c \rho_c} \begin{cases} \ll 1 & \text{one-way coupling} \\ \geq 1 & \text{two-way coupling} \end{cases}$$

Turbulence Modeling in Multiphase Flows

- Turbulence modeling with multiphase flows is challenging.
- Presently, single-phase turbulence models (such as k–ε or RSM) are used to model turbulence in the primary phase only.
- Turbulence equations may contain additional terms to account for turbulence modification by secondary phase(s).
- If phases are separated and the density ratio is of order 1 or if the particle volume fraction is low (< 10%), then a single-phase model can be used to represent the mixture.
- In other cases, either single phase models are still used or “particle-presence-modified” models are used.

Phases as Mixtures of Species

- In all multiphase models within FLUENT, any phase can be composed of either a single material or a mixture of species.
- Material definition of phase mixtures is the same as in single phase flows.
- It is possible to model heterogeneous reactions (reactions where the reactants and products belong to different phases).
  - This means that heterogeneous reactions will lead to interfacial mass transfer.

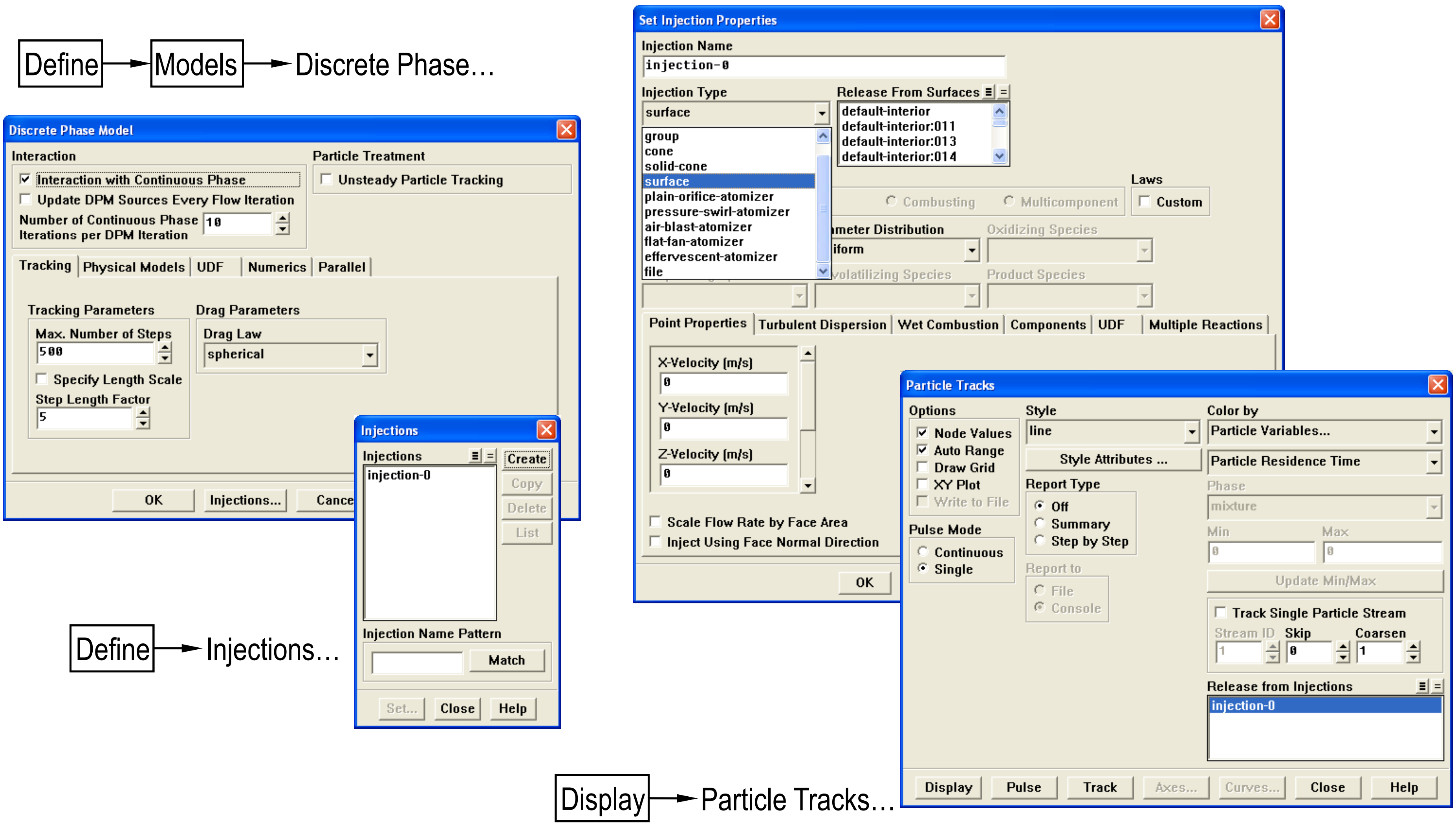
Discrete Phase Model (DPM) Overview

- Trajectories of particles, droplets or bubbles are computed in a Lagrangian frame.
  - Particles can exchange heat, mass, and momentum with the continuous gas phase.
  - Each trajectory represents a group of particles, all with the same initial conditions.
  - DPM neglects collisions and other inter-particle interactions.
  - Turbulent dispersion of particles can be modeled using either stochastic tracking (the most common method) or a particle cloud model.
- Many submodels are available – Heat transfer, vaporization/boiling, combustion, breakup/coalescence, erosion/accretion.

- Applicability of DPM
  - Flow regime: Bubbly flow, droplet flow, particle-laden flow
  - Volume loading: Must be dilute (volume fraction < 12%), otherwise use Dense DPM Model
  - Particulate Loading: Low to moderate
  - Stokes Number: All ranges of Stokes number

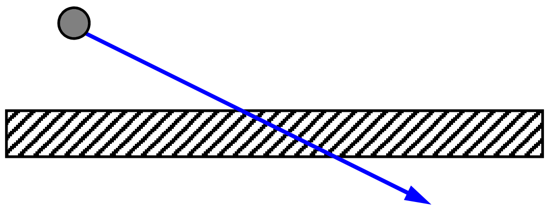
- Application examples
  - Cyclones
  - Spray dryers
  - Particle separation and classification
  - Aerosol dispersion
  - Liquid fuel
  - Coal combustion

Discrete Phase Model (DPM) Setup

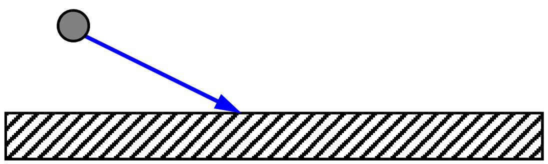


DPM Boundary Conditions

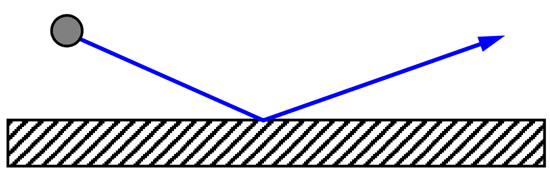
- **Escape**

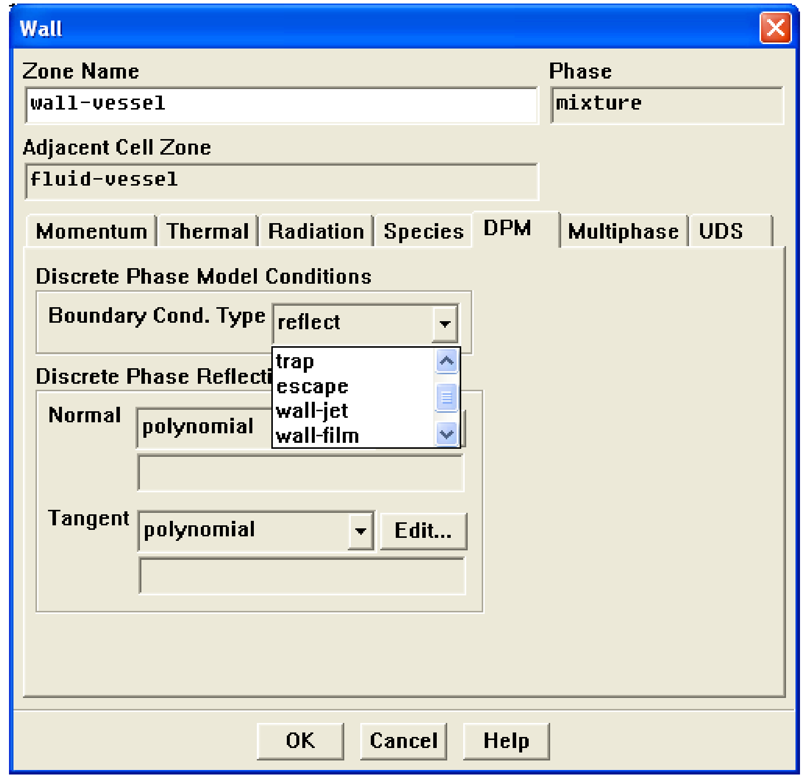


- **Trap**

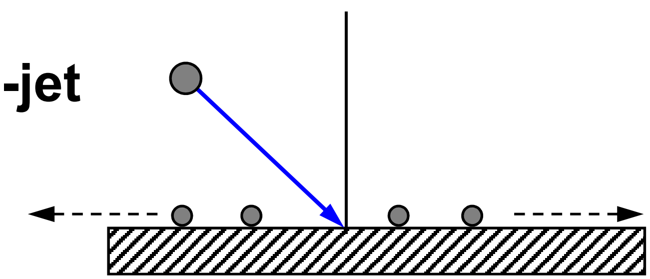


- **Reflect**





- **Wall-jet**



The Eulerian Multiphase Model

- The Eulerian multiphase model is a multi-fluid model. This means that all phases are assumed to exist simultaneously.
  - Conservation equations for each phase contain single-phase terms (pressure gradient, thermal conduction etc.)
  - Conservation equations also contain interfacial terms (drag, lift, mass transfer, etc.).
- Interfacial terms are generally nonlinear and therefore, convergence can sometimes be difficult.
- Eulerian Model 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
  - High particle loading flows
  - Slurry flows
  - Sedimentation
  - Fluidized beds
  - Risers
  - Packed bed reactors

Eulerian Multiphase Model Equations

- **Continuity**:

Volume fraction for the q^{th} phase

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

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

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

Solids pressure term is included for granular model.

- The inter-phase exchange forces are expressed as:

  In general: $\mathbf{F}_{pq} = -\mathbf{F}_{qp}$

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

Exchange coefficient

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

Eulerian Multiphase Model Equations

- Multiphase species transport for species i belonging to mixture of qth phase

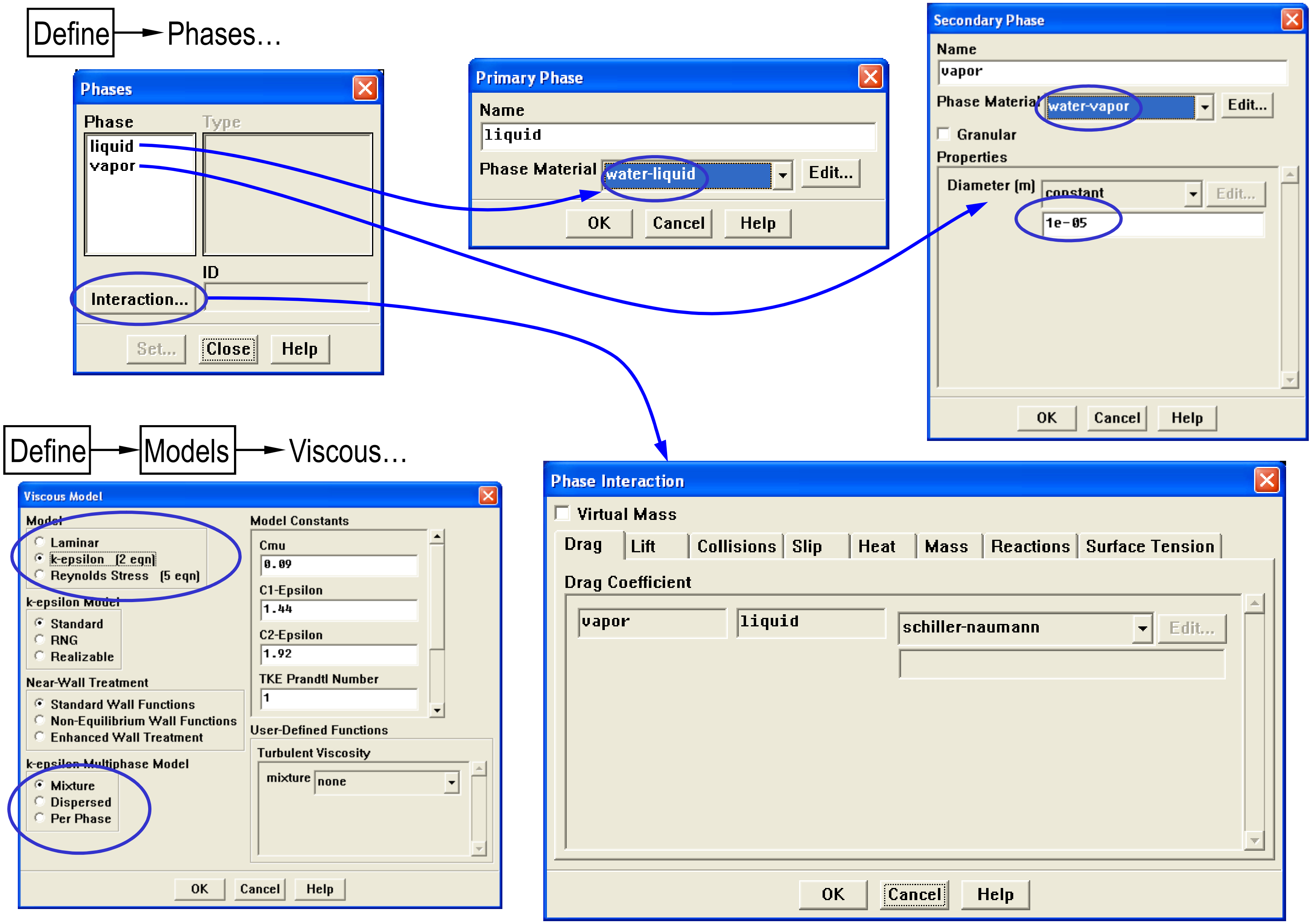
Mass fraction of species *i* in q^{th} phase

$$\underbrace{\frac{\partial}{\partial t}\left(\alpha^q \rho^q Y_i^q\right)}_{\text{transient}} + \underbrace{\nabla \cdot \left(\alpha^q \rho^q \mathbf{u}^q Y_i^q\right)}_{\text{convective}} = \underbrace{-\nabla \cdot \alpha^q \mathbf{J}_i^q}_{\text{diffusion}} + \underbrace{\alpha^q R_i^q}_{\text{homogeneous reaction}} + \underbrace{\alpha^q S_i^q}_{\text{homogeneous production}} + \underbrace{\sum_{p=1}^{n}\left(\dot{m}_{p^i q^j} - \dot{m}_{q^j p^i}\right)}_{\text{heterogeneous reaction}}$$

- Homogeneous and heterogeneous reactions are setup the same as in single phase

- The same species may belong to different phases without any relation between themselves

Eulerian Model Setup



Mixture Model Overview

- The mixture model is a simplified Eulerian approach, based on the assumption of small Stokes number.
  - Solves the mixture momentum equation (for mass-averaged mixture velocity)
  - Solves a volume fraction transport equation for each secondary phase.

- Mixture model applicability
  - Flow regime: Bubbly, droplet, and slurry flows
  - Volume loading: Dilute to moderately dense
  - Particulate Loading: Low to moderate
  - Stokes Number: St << 1

- Application examples
  - Hydrocyclones
  - Bubble column reactors
  - Solid suspensions
  - Gas sparging

Mixture Model Equations

- Solves one equation for continuity of the mixture

$$\frac{\partial \rho_m}{\partial t} + \nabla \cdot (\rho_m \mathbf{u}_m) = \dot{m}$$

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

$$\frac{\partial \alpha_k \rho_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_m) = -\nabla \cdot \left(\alpha_k \rho_k \mathbf{u}_k^r \right)$$

Drift velocity

$$\mathbf{u}_k^r = \mathbf{u}_k - \mathbf{u}_m$$

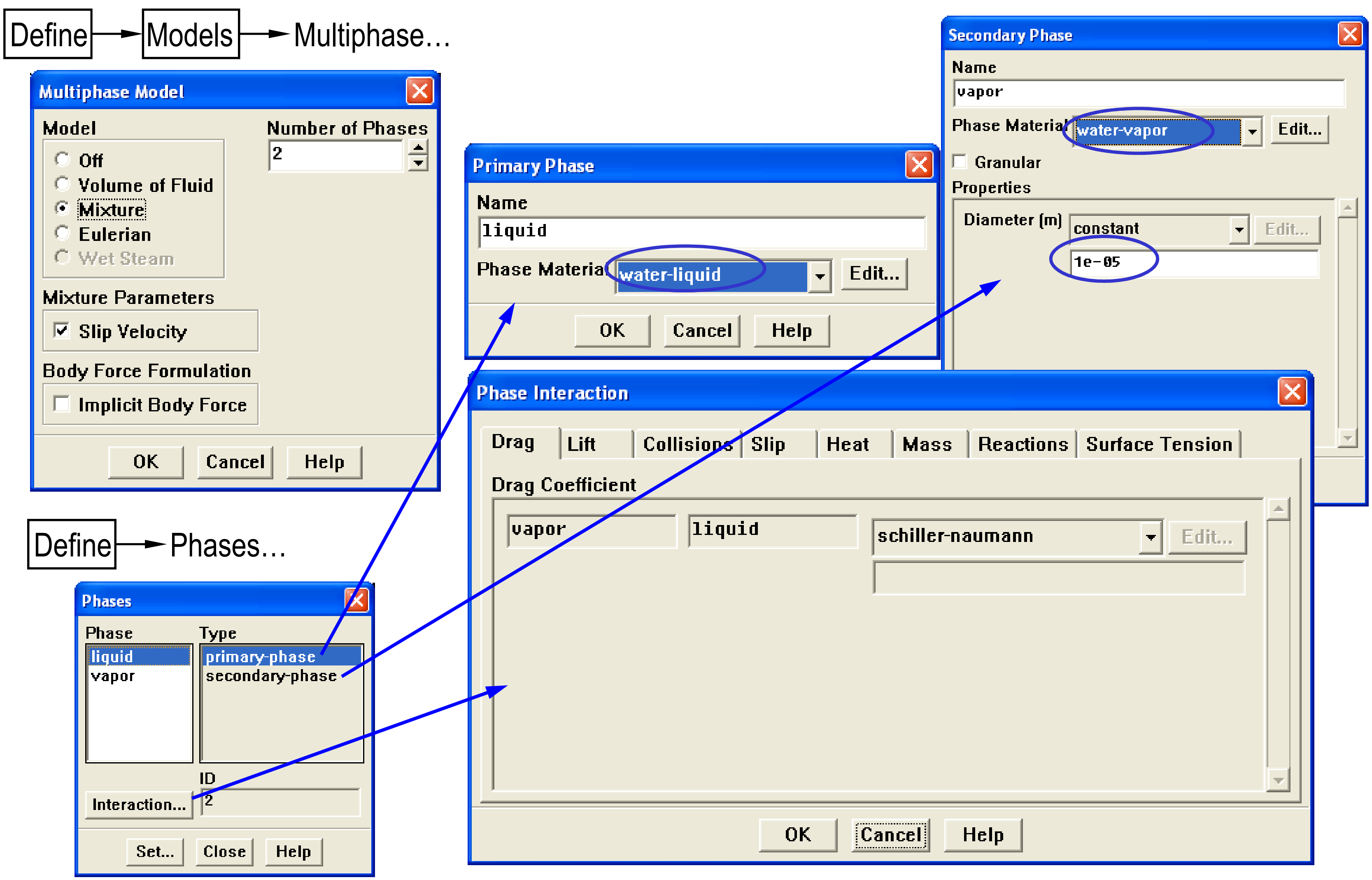
- Solves one equation for the momentum of the mixture

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

- The mixture properties are defined as:

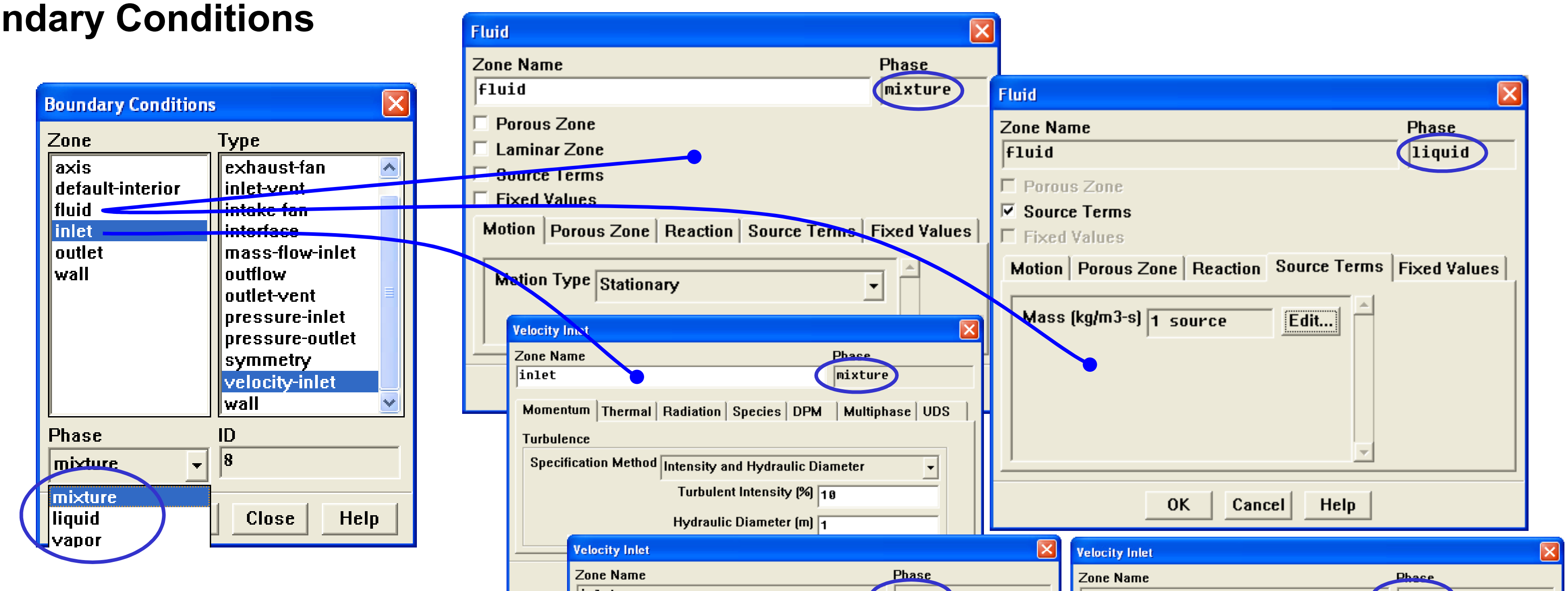
$$\rho_m = \sum_{k=1}^{n} \alpha_k \rho_k \qquad \mu_m = \sum_{k=1}^{n} \alpha_k \mu_k \qquad \mathbf{u}_m = \frac{1}{\rho_m} \sum_{k=1}^{n} \alpha_k \rho_k \mathbf{u}_k$$

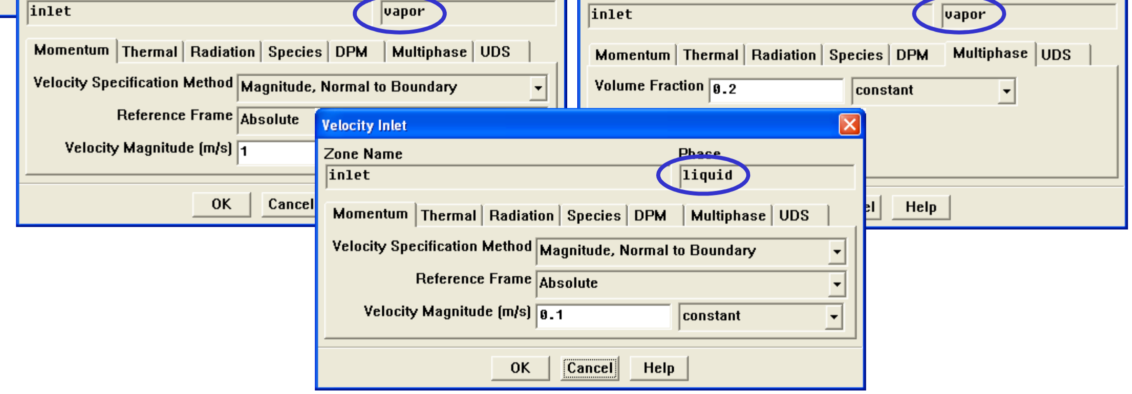
Mixture Model Setup



Mixture Model Setup

- **Boundary Conditions**

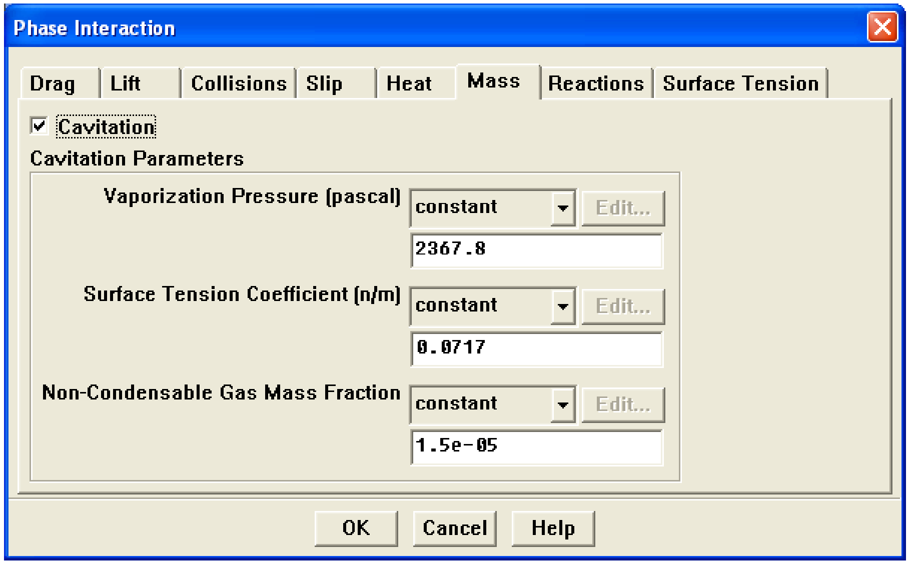




- **Volume fraction defined for each secondary phase.**
- **To define initial phase location, patch volume fractions after solution initialization.**

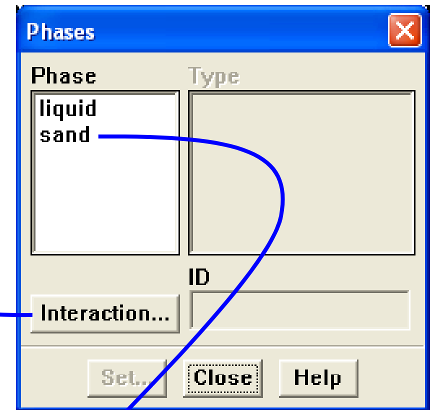
Cavitation Submodel

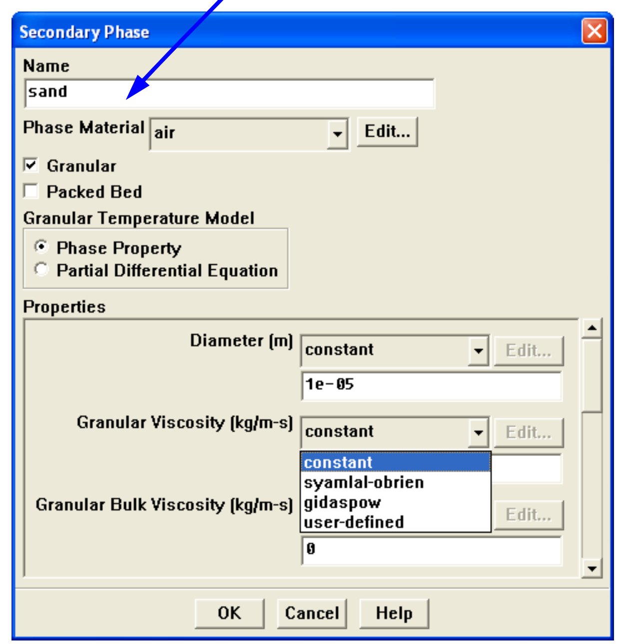
- The Cavitation model models the formation of bubbles when the local liquid pressure is below the vapor pressure.
- The effect of non-condensable gases is included.
- Mass conservation equation for the vapor phase includes vapor generation and condensation terms which depend on the sign of the difference between local pressure and vapor saturation pressure (corrected for on-condensable gas presence).
- Generally used with the mixture model, incompatible with VOF.
- Tutorial is available for learning the in-depth setup procedure.

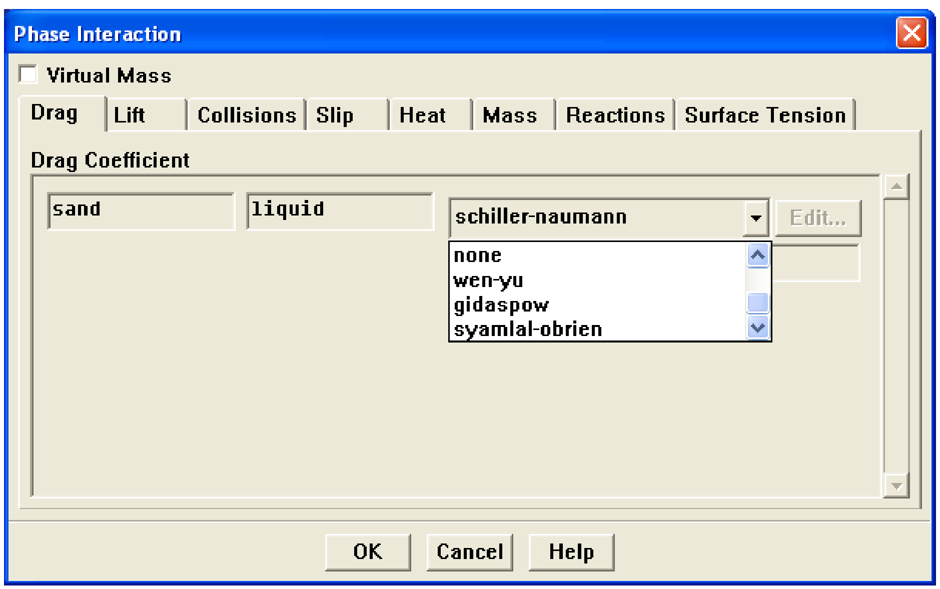


Eulerian-Granular Model Setup

- Granular option must be enabled when defining the secondary phases.
- Granular properties require definition.
- Phase interaction models appropriate for granular flows must be selected.







The Volume of Fluid (VOF) Model Overview

- The VOF model is designed to track the location and motion of a free surface between two or more immiscible fluids.

- VOF model can account for:
  - Turbulence, energy and species transport
  - Surface tension and wall adhesion effects.
  - Compressibility of phase(s)

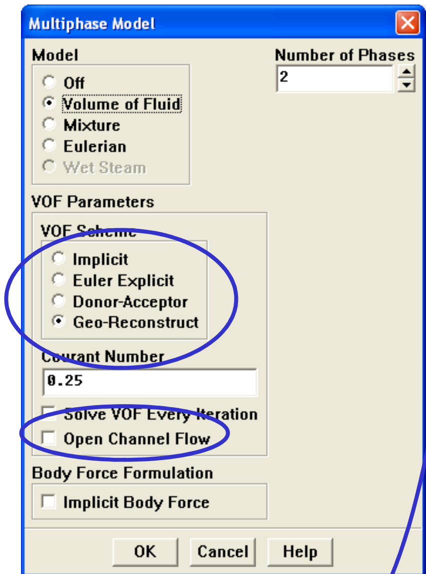
- VOF model applicability:

– Flow regime	Slug flow, stratified/free-surface flow
– Volume loading	Dilute to dense
– Particulate loading	Low to high
– Turbulence modeling	Weak to moderate coupling between phases
– Stokes number	All ranges

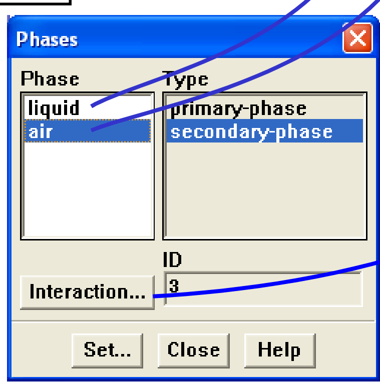
- Application examples
  - Large slug flows
  - Tank filling
  - Offshore separator sloshing
  - Coating

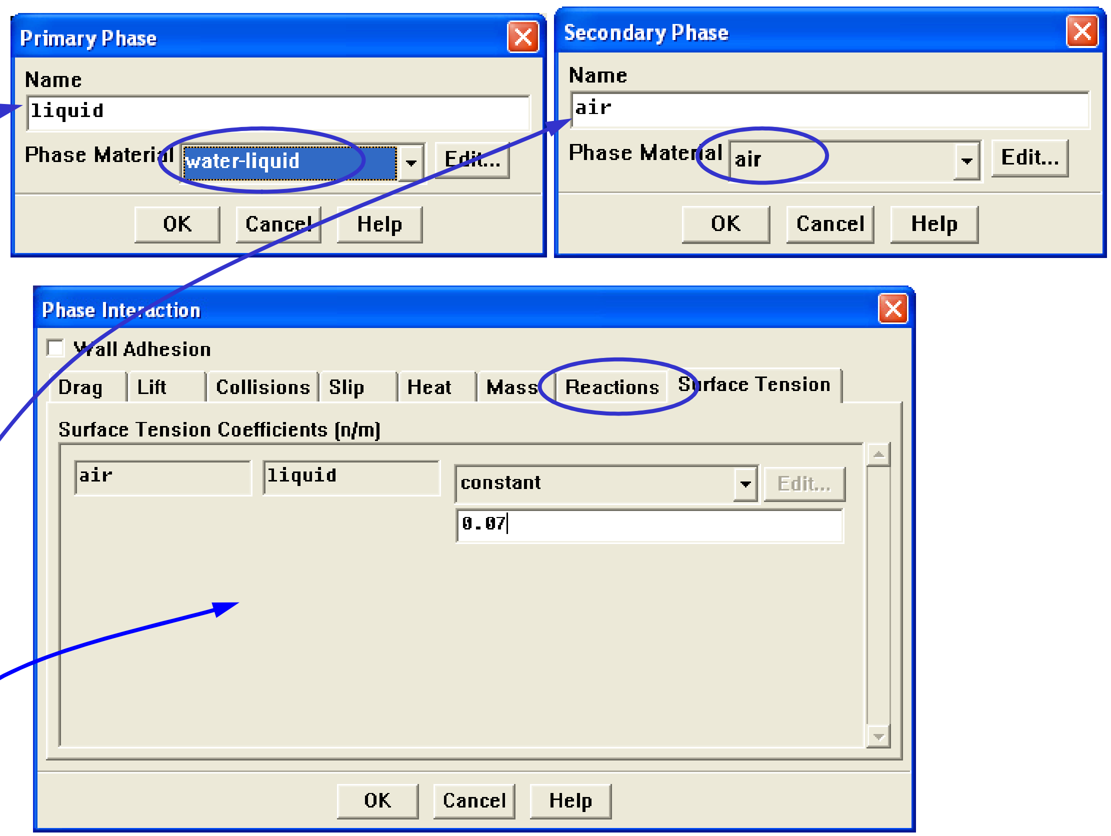
VOF Model Setup

Define → Models → Multiphase…



Define → Phases…



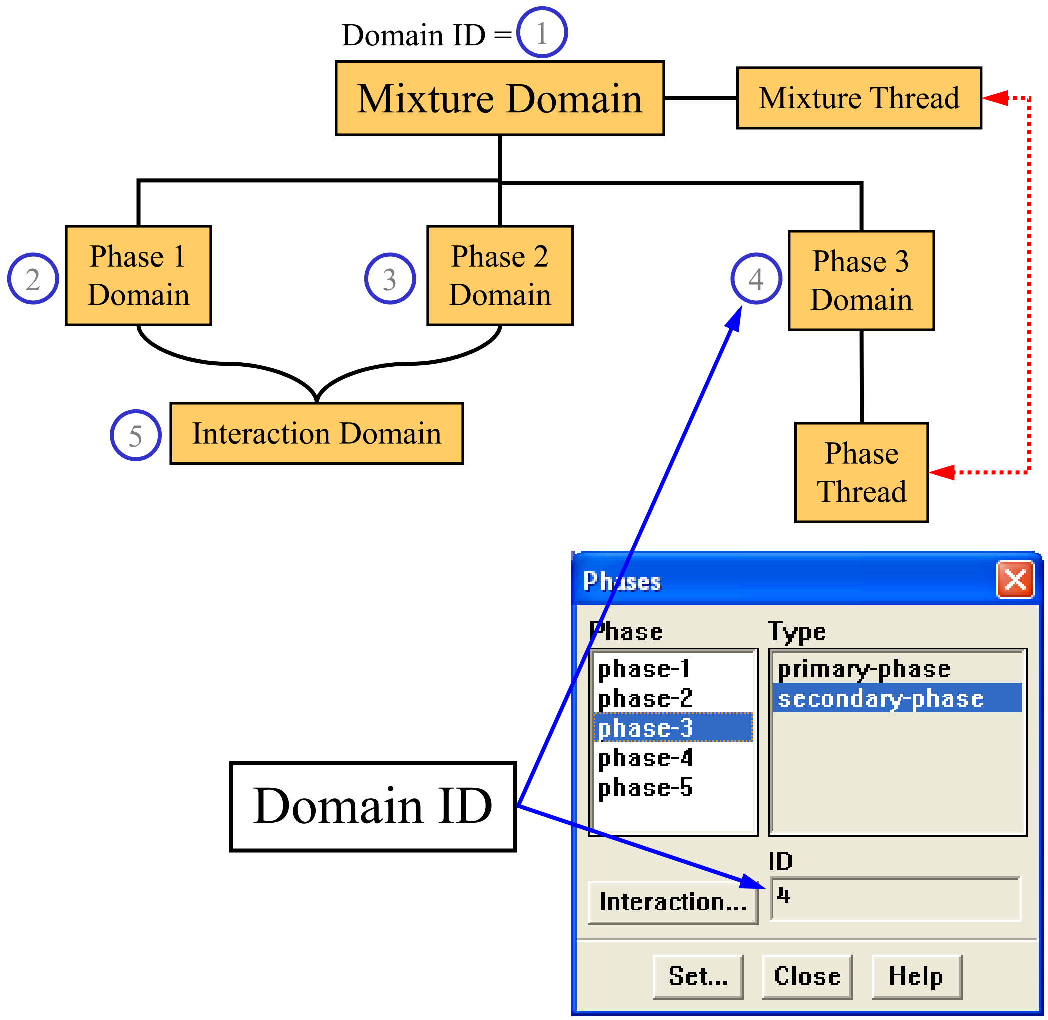


Define → Operating Conditions…

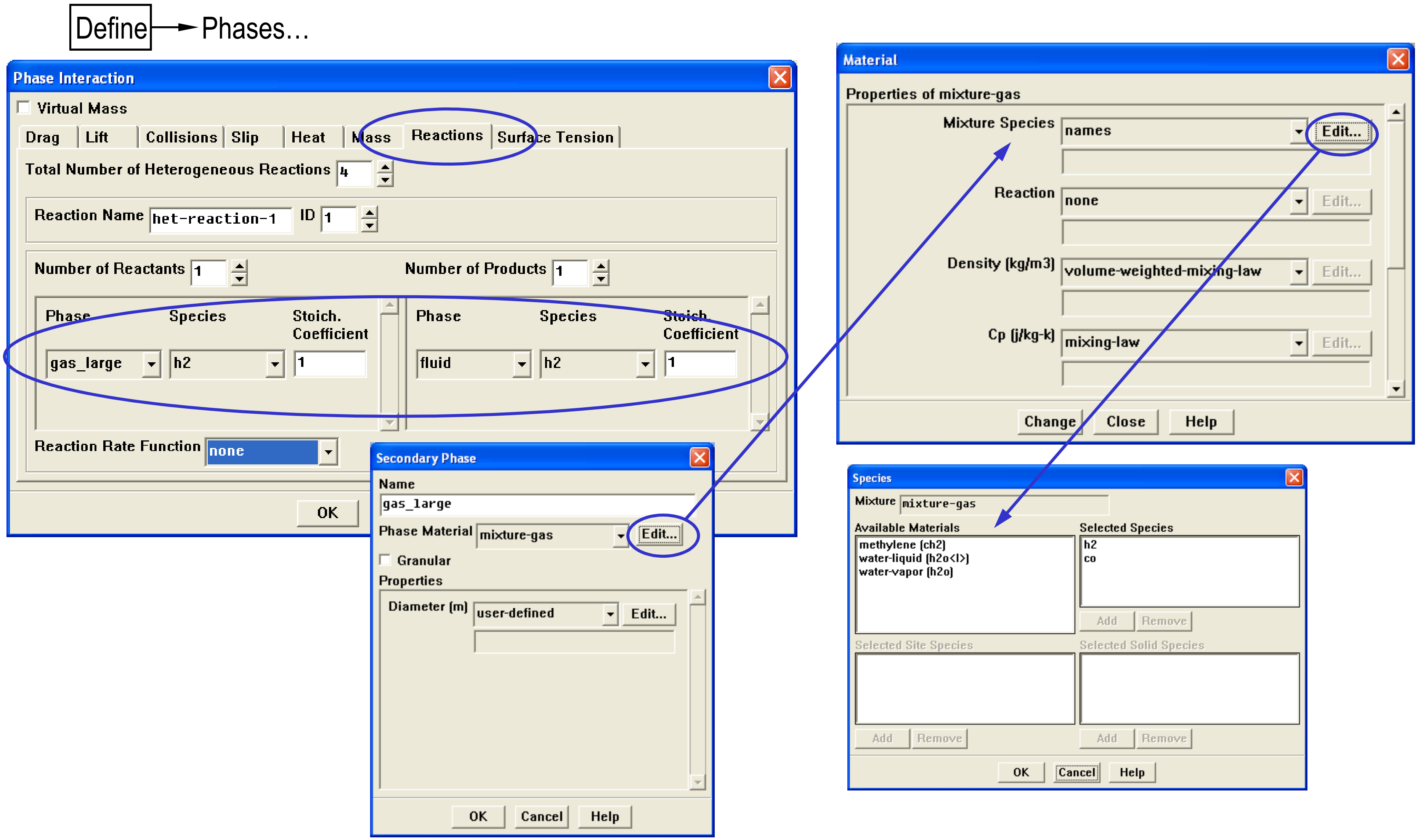
Operating Density should be set to that of lightest phase with body forces enabled.

UDFs for Multiphase Applications

- When a multiphase model is enabled, storage for properties and variables is set aside for mixture as well as for individual phases.
  - Additional thread and domain data structures required.
- In general the type of `DEFINE` macro determines which thread or domain (mixture or phase) gets passed to your UDF.
- `C_R(cell,thread)` will return the *mixture* density if `thread` is the *mixture* thread or the *phase* densities if it is the *phase* thread.
- Numerous macros exist for data retrieval.



Heterogeneous Reaction Setup



Appendix 2

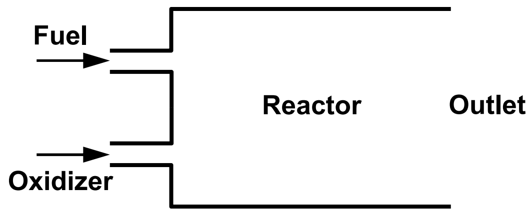
Reacting Flow Modeling

Eddy Dissipation Model (EDM)

- Applicability
  - Flow Regime: Turbulent flow (high Re)
  - Chemistry: Fast chemistry
  - Configuration: Premixed / Non-Premixed / Partially Premixed
- Application examples
  - Gas reactions
  - Coal combustion
- Limitations
  - Unreliable when mixing and kinetic time scales are of similar order of magnitude
  - Does not predict kinetically-controlled intermediate species and dissociation effects.
  - Cannot realistically model phenomena which depend on detailed kinetics such as ignition, extinction.
- Solves species transport equations. Reaction rate is controlled by turbulent mixing.

Non-Premixed Model

- Applicability
  - Flow Regime: Turbulent flow (high Re)
  - Chemistry: Equilibrium or moderately non-equilibrium (flamelet)
  - Configuration: Non-Premixed only



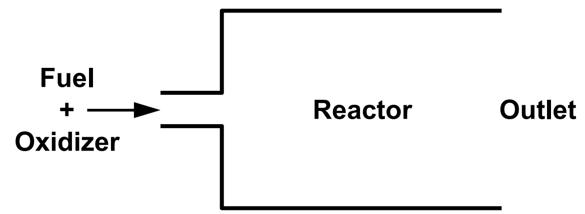
- Application examples
  - Gas reaction (furnaces, burners). This is usually the model of choice if assumptions are valid for gas phase combustion problems. Accurate tracking of intermediate species concentration and dissociation effects without requiring knowledge of detailed reaction rates (equilibrium).

- Limitations
  - Unreliable when mixing and kinetic time scales are comparable
  - Cannot realistically model phenomena which depend on detailed kinetics (such as ignition, extinction).

- Solves transport equations for mixture fraction and mixture fraction variance (instead of the individual species equations).

Premixed Combustion Model

- Applicability
  - Flow Regime: Turbulent flow (high Re)
  - Chemistry: Fast chemistry
  - Configuration: Premixed only



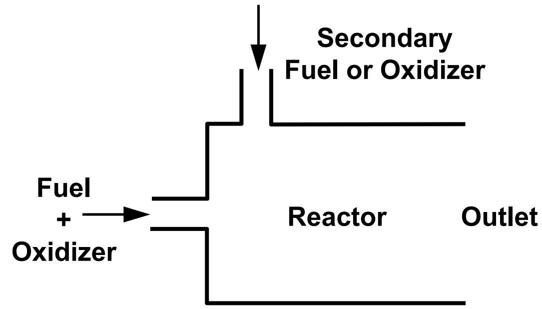
- Application examples
  - Premixed reacting flow systems
  - Lean premixed gas turbine combustion chamber

- Limitations
  - Cannot realistically model phenomena which depend on detailed kinetics (such as ignition, extinction).

- Uses a reaction progress variable which tracks the position of the flame front (Zimont model).

Partially Premixed Combustion Model

- Applicability
  - Flow Regime: Turbulent flow (high Re)
  - Chemistry: Equilibrium or moderately non-equilibrium (flamelet)
  - Configuration: Partially premixed only



- Application examples
  - Gas turbine combustor with dilution cooling holes.
  - Systems with both premixed and non-premixed streams

- Limitations
  - Unreliable when mixing and kinetic time scales are comparable.
  - Cannot realistically model phenomena which depend on detailed kinetics (such as ignition, extinction).

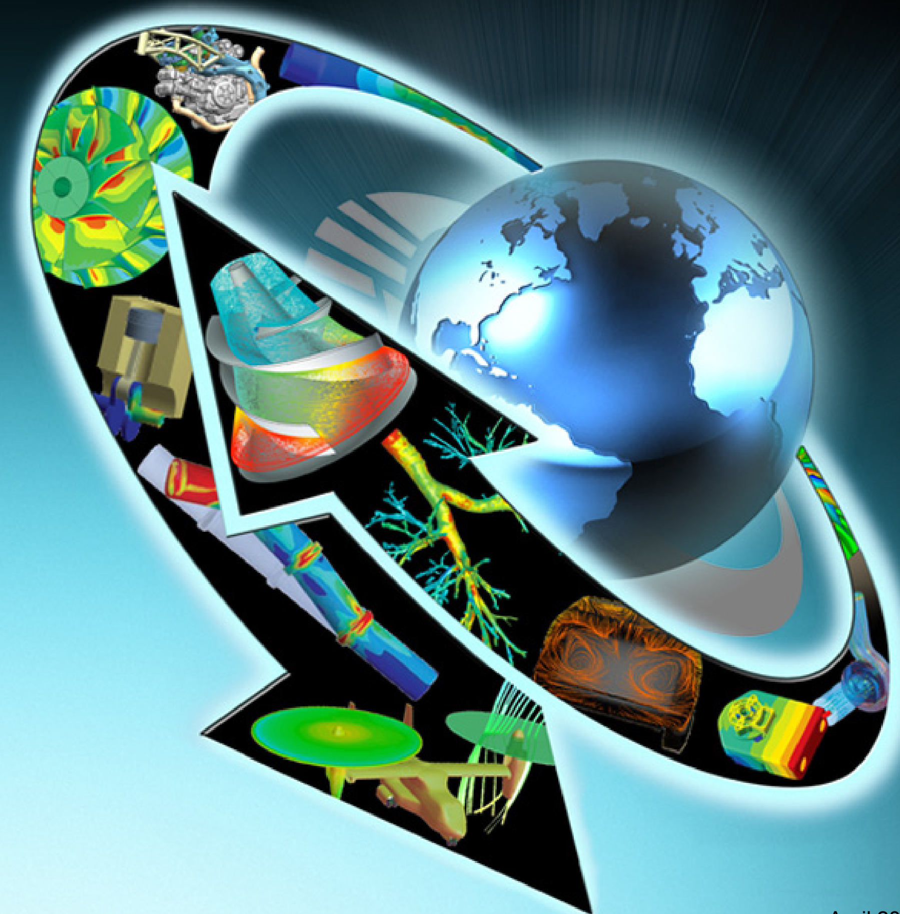
- In the partially premixed model, reaction progress variable and mixture fraction approach are combined. Transport equations are solved for reaction progress variable, mixture fraction, and mixture fraction variance.

Detailed Chemistry Models

- The governing equations for detailed chemistry are generally stiff and difficult to solve.
  - Tens of species
  - Hundreds of reactions
  - Large spread in reaction time scales.
- Detailed kinetics are used to model:
  - Flame ignition and extinction
  - Pollutants (NOx, CO, UHCs)
  - Slow (non-equilibrium) chemistry
  - Liquid/liquid reactions
- Available Models:
  - Laminar finite rate
  - Eddy Dissipation Concept (EDC) Model
  - PDF transport
  - KINetics model (requires additional license feature)
- CHEMKIN-format reaction mechanisms and thermal properties can be imported directly.
- FLUENT uses the In-Situ Adaptive Tabulation (ISAT) algorithm in order to accelerate calculations (applicable to laminar, EDC, PDF transport models).

Appendix 3

Moving and Deforming Mesh



Absolute and Relative Velocities – The Velocity Triangle

- Absolute Velocity – velocity measured w.r.t. the stationary frame
- Relative Velocity – velocity measured w.r.t. the moving frame.

- The relationship between the absolute and relative velocities is given by the Velocity Triangle rule:

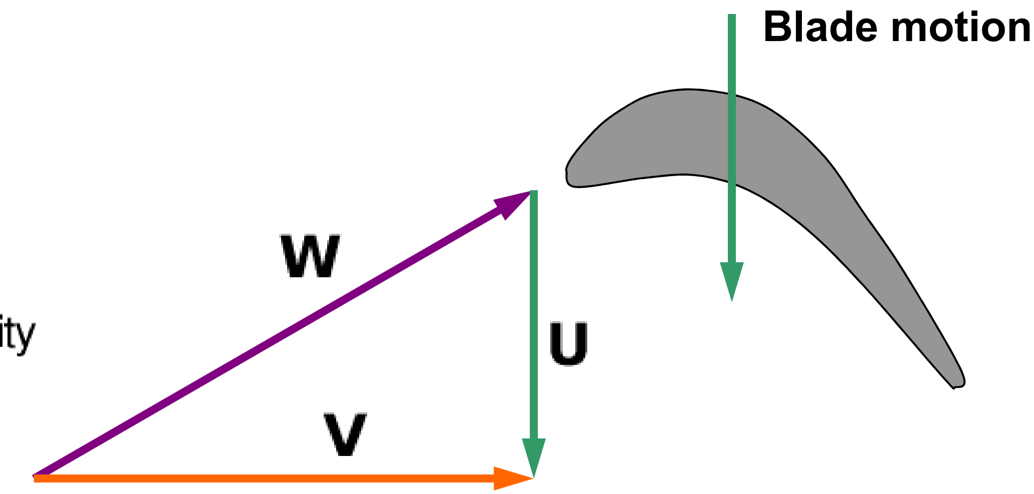
$$\mathbf{V} = \mathbf{W} + \mathbf{U}$$

- In turbomachinery, this relationship can be illustrated using the laws of vector addition.

$\mathbf{V}$ = Absolute velocity

$\mathbf{W}$ = Relative velocity

$\mathbf{U}$ = Moving frame velocity

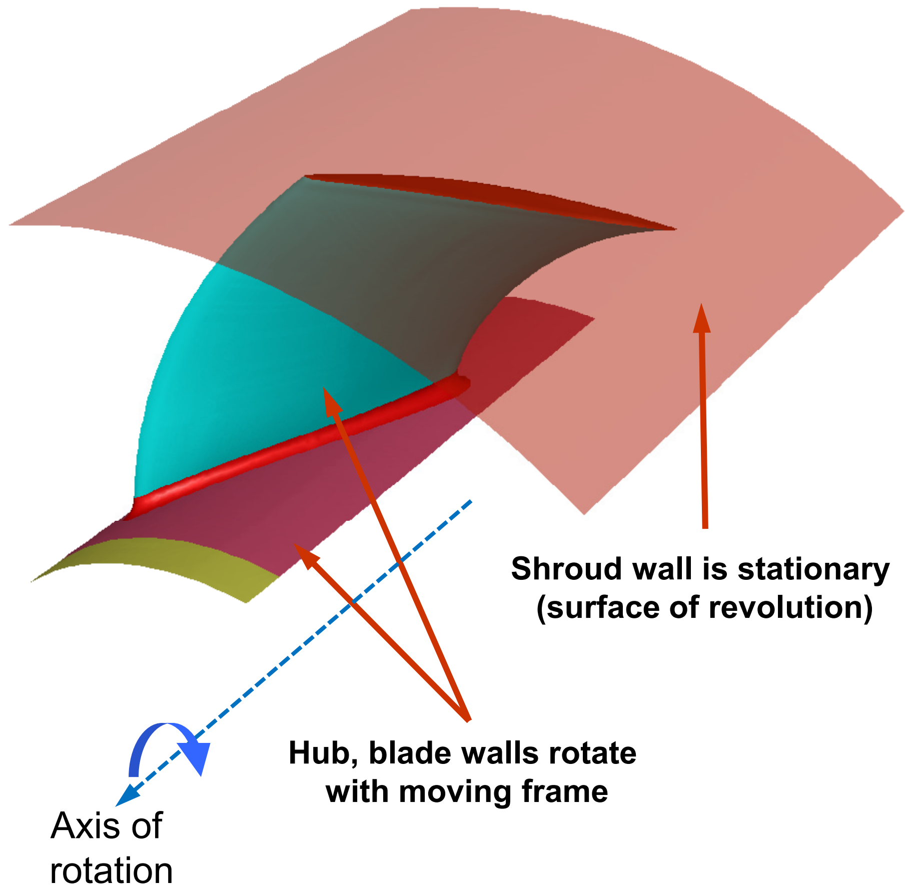


Geometry Constraints for SRF

- Single Fluid Domain

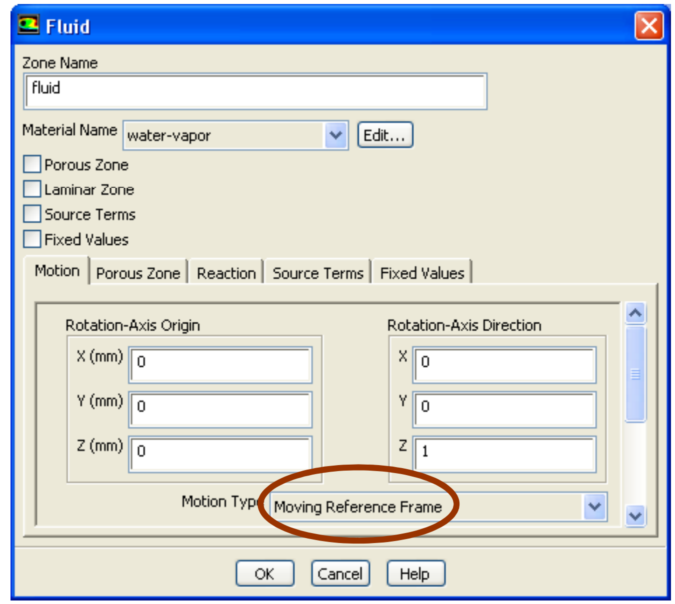
- Walls and flow boundaries
  - Walls and flow boundaries (inlets and outlets) which move with the fluid domain may assume any shape.
  - Walls and flow boundaries which are stationary (with respect to the fixed frame) must be surfaces of revolution about the rotational axis.
  - You can also impose a tangential component of velocity on a wall provided the wall is a surface of revolution.

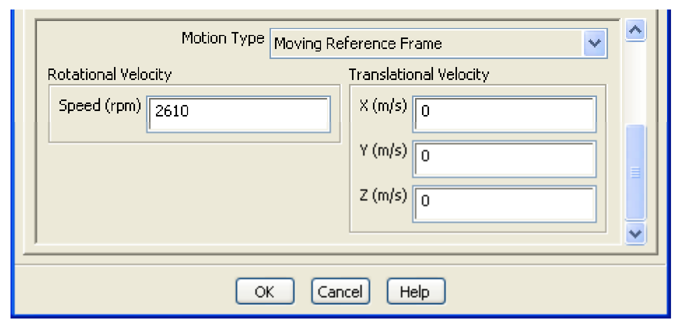
- You can employ rotationally-periodic boundaries if geometry and flow permit
  - Advantage - reduced domain size



SRF Set-up: Cell Zones

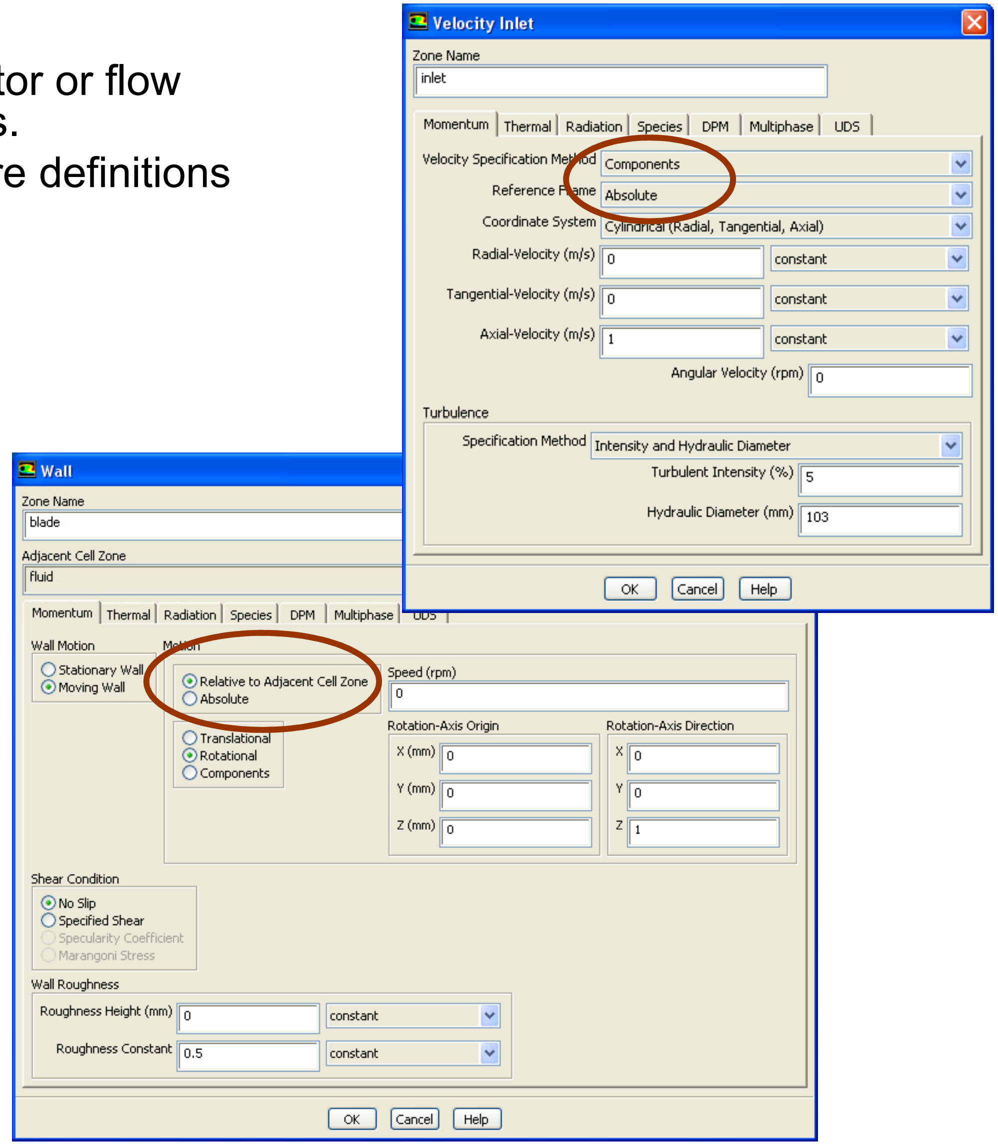
- Use fluid BC panel to define rotational axis origin and direction vector for rotating reference frame
  - Direction vectors should be unit vectors but Fluent will normalize them if they aren’t
- Select <u>Moving Reference Frame</u> as the Motion Type for SRF
- Enter Moving Frame Velocities
  - Rotational and Translational velocities
  - Rotation direction defined by right-hand rule
  - Negative speed implies rotation in opposite direction





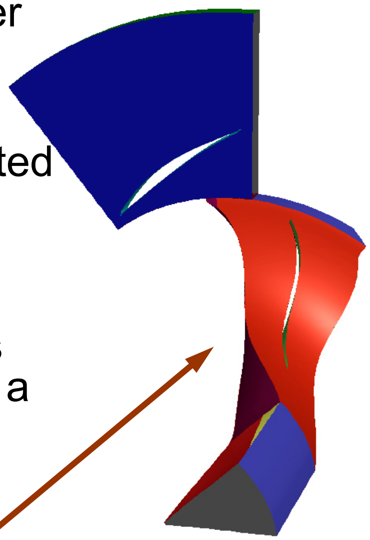
SRF Set-up: Boundary Conditions

- Inlets:
  - Choice of specification of velocity vector or flow direction in absolute or relative frames.
  - NOTE: Total pressure and temperature definitions depend on velocity formulation!
- Outlets
  - Static pressure or outflow.
  - Radial equilibrium option.
- Other Flow BCs
  - Periodics
  - Non-reflecting BCs
  - Target mass flow outlet
- Walls
  - Specify walls to be…
    - Moving with the domain
    - Stationary
  - NOTE: “Stationary wall” for Wall Motion means stationary w.r.t. the cell zone!

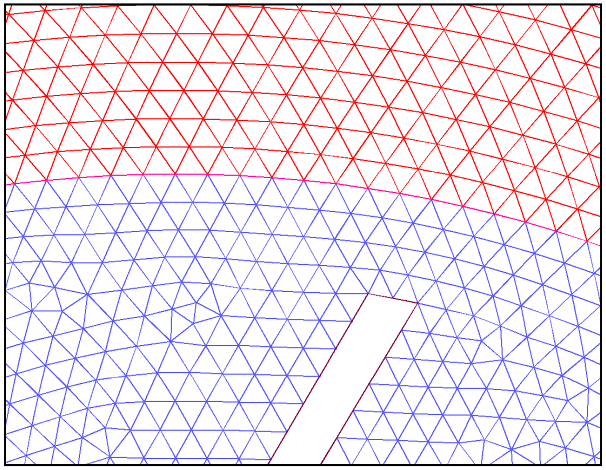


Interfaces

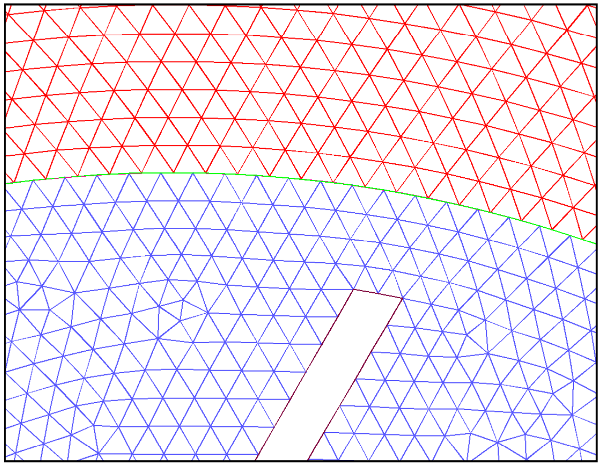
- Fluid zones in multiple zone models communicate across **interface** boundaries.
- Conformal interfaces
  - An interior mesh surface separates cells from adjacent fluid zones.
  - Face mesh must be identical on either side of the interface.
- Non-conformal (NC) interfaces
  - Cells zones are physically disconnected from each other.
  - Interface consists of <u>two</u> overlapping surfaces (type = interface)
  - Fluent NC interface algorithm passes fluxes from on surface to the other in a conservative fashion (i.e. mass, momentum, energy fluxes are conserved).
  - User creates interfaces using Define→Grid Interfaces…
- Interfaces may be periodic
  - Called periodic repeat interface.
  - Require <u>identical</u> translational or rotational offset.



Periodic repeat interface



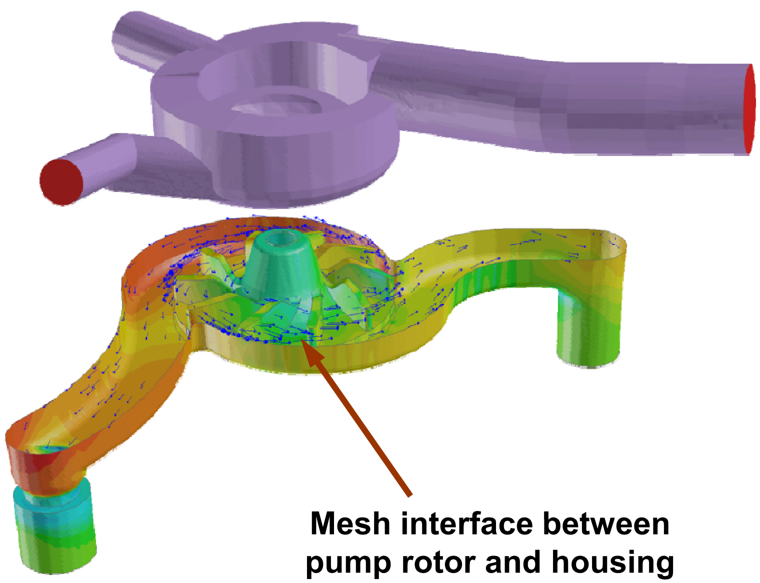
Conformal interface



Non-conformal interface

The MRF Model

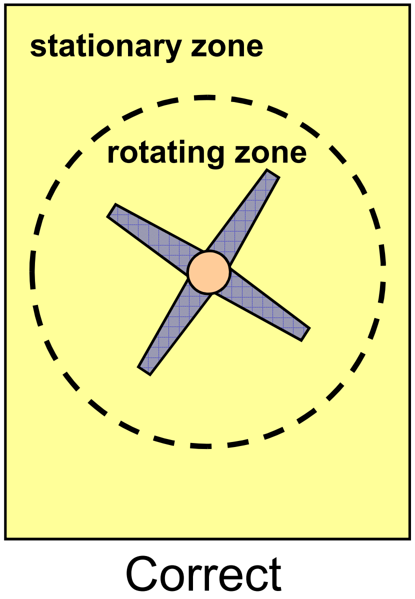
- The computational domain is divided into stationary and rotating fluid zones.
  - Interfaces separate zones from each other.
  - Interfaces can be Conformal or Non-Conformal.
- Flow equations are solved in each fluid zone.
  - Flow is assumed to be steady in each zone (clearly an approximation).
  - SRF equations used in rotating zones.
  - At the interfaces between the rotating and stationary zones, appropriate transformations of the velocity vector and velocity gradients are performed to compute fluxes of mass, momentum, energy, and other scalars.
- MRF ignores the relative motions of the zones with respect to each other.
  - Does not account for fluid dynamic interaction between stationary and rotating components.
  - For this reason MRF is often referred to as the "frozen rotor" approach.
- Ideally, the flow at the MRF interfaces should be relatively uniform or "mixed out."

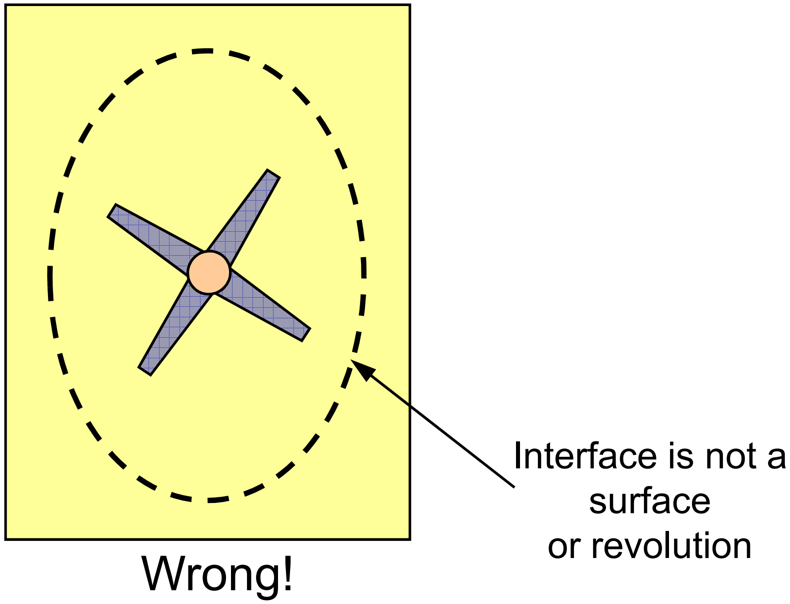


Mesh interface between pump rotor and housing

Geometric Constraints for MRF

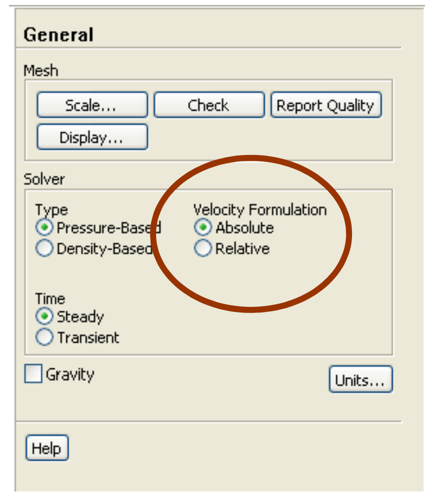
- Walls and flow boundaries which are contained within the rotating fluid zone interfaces are assumed to be moving with the fluid zones and may assume any shape.
  - Stationary walls and flow boundaries are allowed if they are surfaces of revolution.
- The interface between two zones must be a surface of revolution with respect to the axis of rotation of the rotating zone.
- Periodic repeat interfaces are permitted but the periodic angles (or offsets) must be identical for all zones.





Equations of Fluid Dynamics for Moving Frames

- Equations of fluid dynamics can be transformed to a moving reference frame with a choice of the velocities which are solved.
  - Relative Velocity Formulation (RVF)
    - Uses the relative velocity and relative total internal energy as the dependent variables.
  - Absolute Velocity Formulation (AVF)
    - Uses the relative velocity and relative total internal energy as the dependent variables.



- Source terms appear in the momentum equations for rotating frames.
  - Refer to Appendix for detailed listing of equations.
  - Relative formulation of x momentum equation:

$$\frac{\partial(\rho w_x)}{\partial t} + \nabla\cdot\rho\mathbf{W}w_x = -\frac{\partial p}{\partial x} + \nabla\cdot\tau_{vrx} - \boxed{\rho(2\boldsymbol{\omega}\times\mathbf{W} + \boldsymbol{\omega}\times\boldsymbol{\omega}\times\mathbf{r})\cdot\mathbf{i}}$$

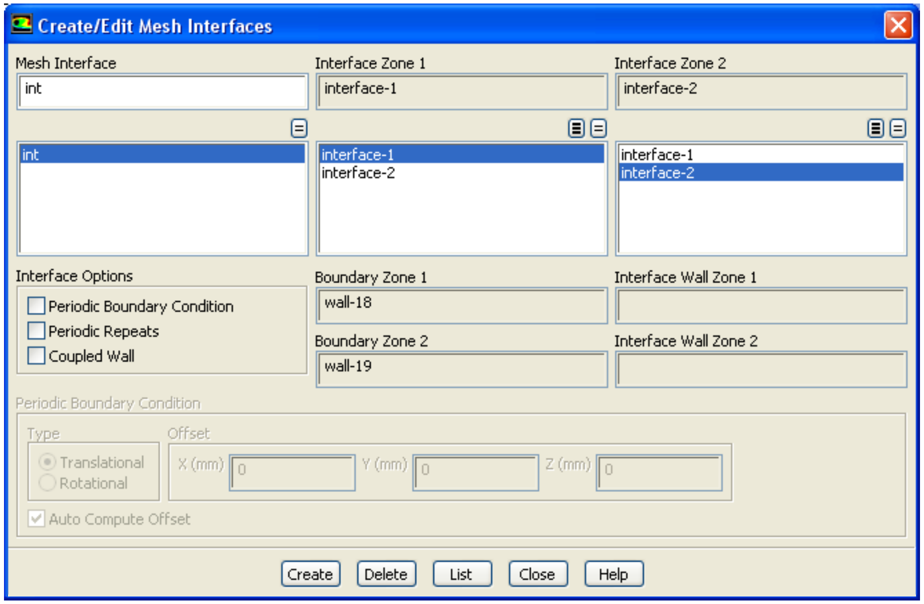
  - Absolute formulation of x momentum equation:

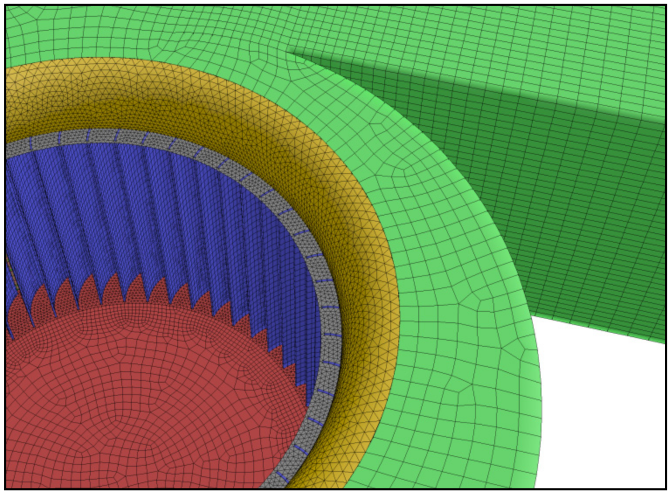
$$\frac{\partial(\rho v_x)}{\partial t} + \nabla\cdot\rho\mathbf{W}v_x = -\frac{\partial p}{\partial x} + \nabla\cdot\tau_{vx} - \boxed{\rho(\boldsymbol{\omega}\times\mathbf{v})\cdot\mathbf{i}}$$

Momentum source terms

MRF Set-Up

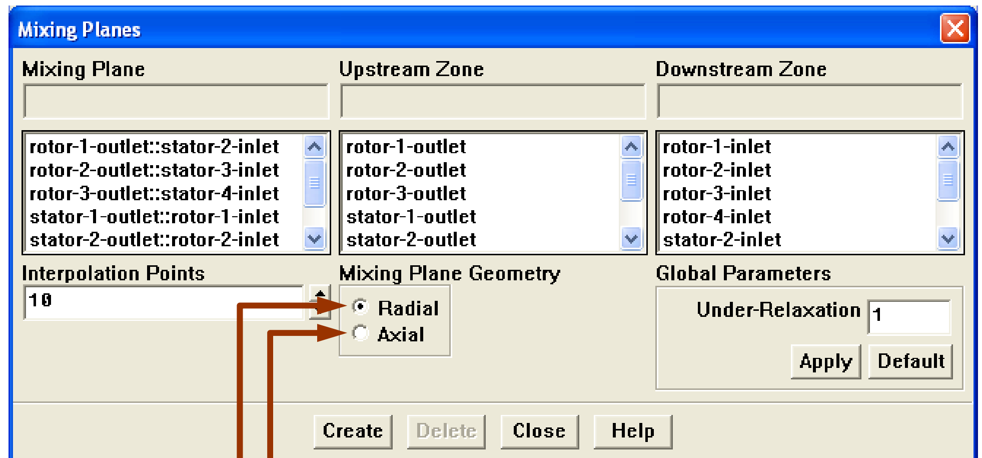
- Generate mesh with appropriate stationary and rotating fluid zones
  - Can choose conformal or non-conformal interfaces between cell zones
- For each rotating fluid zone (Fluid BC), select "Moving Reference Frame" as the Motion Type and enter the rotational axis and moving frame speed.
  - Identical to SRF except for multiple zones
  - Stationary zones remain with "Stationary" option enabled
- Set up for BCs and solver settings same as SRF.





MPM Set-up

- Assign motion types and speeds to fluid zones and appropriate BCs for each zone (like SRF).
- Select upstream and downstream zones which will comprise mixing plane pair.
  - Upstream will always be Pressure Outlet.
  - Downstream can be any inlet BC type.
- Set the number of Interpolation Points for profile resolution.
  - Should be about the same axial/radial resolution as the mesh.
- Mixing Plane Geometry determines method of profile averaging.
- Mixing plane controls
  - Under-relaxation – Profile changes are under-relaxed from one iteration to the next using factor between 0 and 1.

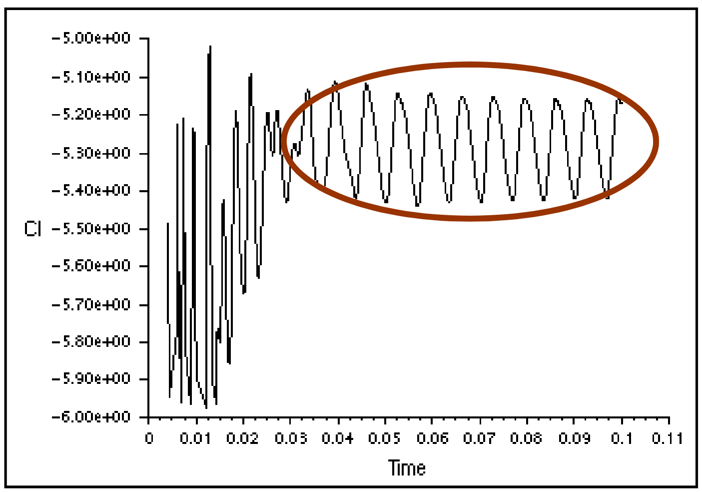


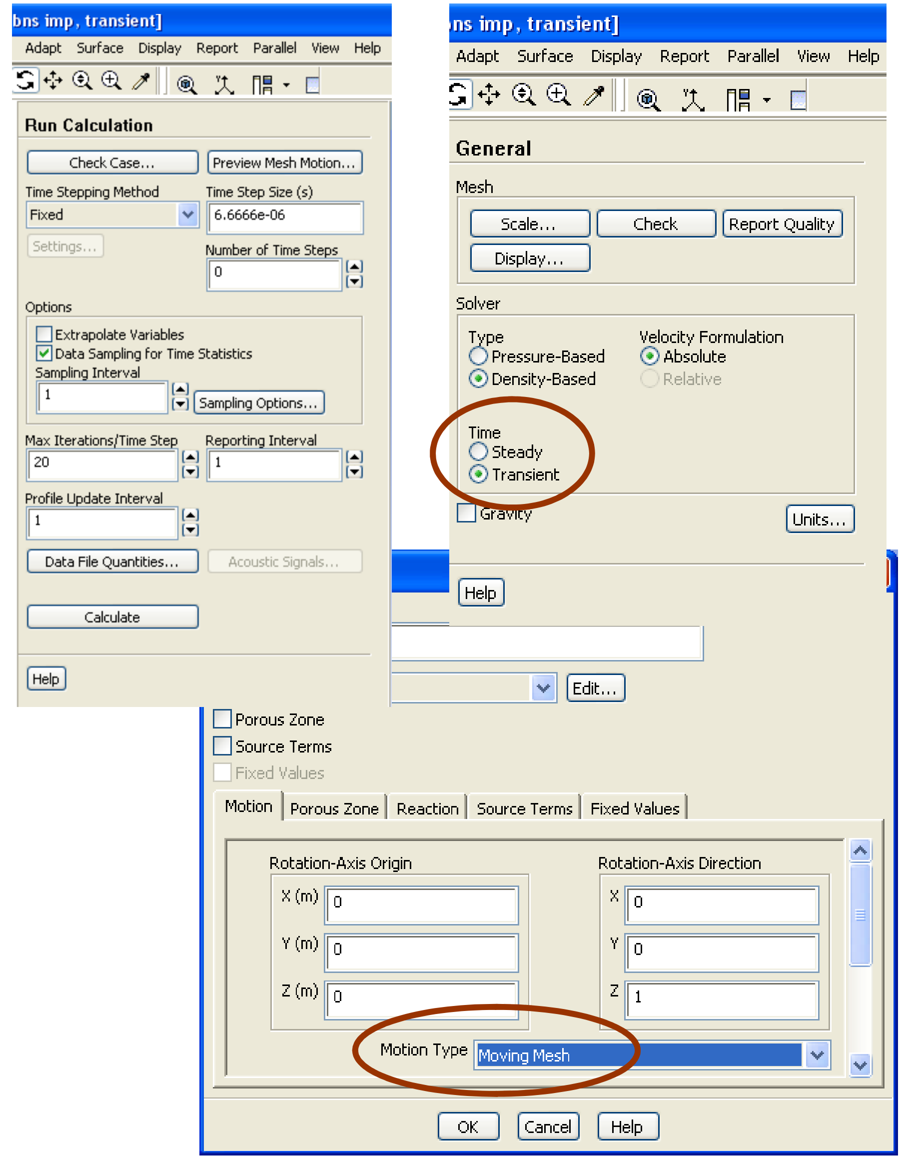
$$\bar{\phi}_z(r) = \frac{1}{\Delta\theta_p} \int_{\Delta\theta_p} \phi(r,\theta)\, d\theta$$

$$\bar{\phi}_r(z) = \frac{1}{\Delta\theta_p} \int_{\Delta\theta_p} \phi(z,\theta)\, d\theta$$

SMM Set-up

- Enable transient solver.
- For moving zones, select Moving Mesh as Motion Type in Fluid BC panel.
- Define sliding zones as non-conformal interfaces.
  - Enable Periodic Repeat option if sliding/rotating motion is periodic.
- Other BCs and solver settings are same as the SRF, MRF models.
- Run calculation until solution becomes time-periodic





Dynamic Mesh Setup

- Enable transient solver.
- Enable Dynamic Mesh model in Define→Dynamic Mesh.
- Activate desired Mesh Methods and set parameters as appropriate.
- Define boundary motion in the Dynamic Mesh Zones GUI.
  - UDF may be required.
- Other models, BCs, and solver settings are same as SMM models.
- Mesh motion can be previewed using Solve→Mesh Motion utility.