

Advanced Physics

Introduction

Lecture Theme:

Fluent offers extensive capabilities for multiphase flow and combustion modeling. This lecture will familiarize you with Fluent's models, our advanced training course offerings and additional knowledge resources available on the Customer Portal

Learning Aims:

You will learn:

- Basics of multiphase flows
- Multiphase models available in Fluent and how to choose which model to use
- Basics of reacting flows
- Combustion models available in Fluent and how to choose which model to use

Learning Objectives:

Basic understanding of Fluent's multiphase and combustion models and additional training and knowledge resources

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Advanced Physics

Outline

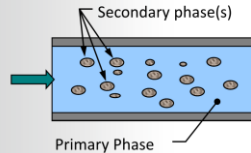
- **Multiphase Flow Modeling**
 - Discrete phase model
 - Eulerian model
 - Mixture model
 - Volume-of-fluid model
- **Reacting Flow Modeling**
 - Eddy dissipation model
 - Non-premixed, premixed and partially premixed combustion models
 - Detailed chemistry models
 - Pollutant formation
 - Surface reactions

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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)



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)*

Introduction

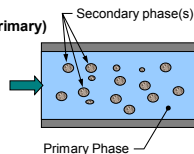
- A phase is a class of matter with a **definable boundary** and a particular dynamic response to the surrounding flow/potential field.

- Phases are generally identified by solid, liquid or gas, but can also refer to other forms:

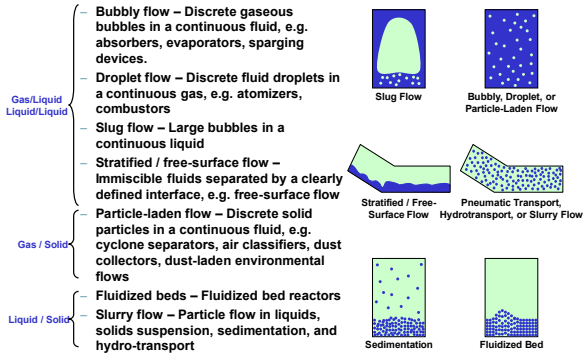
- Materials with different chemical properties but in the same state or phase (i.e. liquid-liquid)

- The fluid system is defined by a primary and multiple secondary phases.

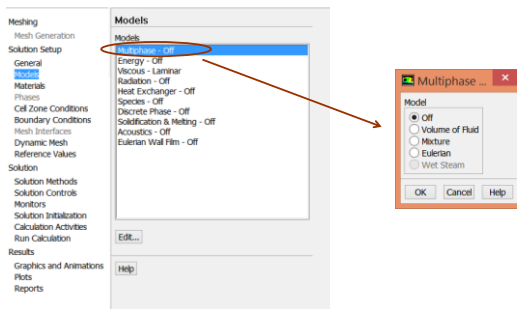
- One of the phases is considered continuous (primary)
- The others (secondary) are considered to be dispersed within the continuous phase.
- There may be several secondary phase denoting particles of with different sizes.



Multiphase Flow Regimes

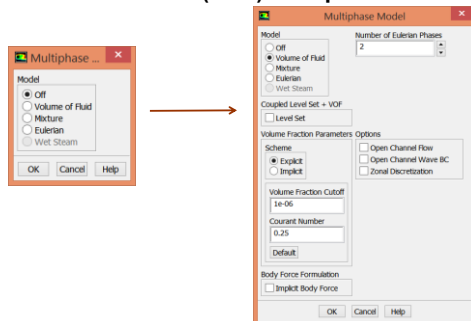


Multiphase models

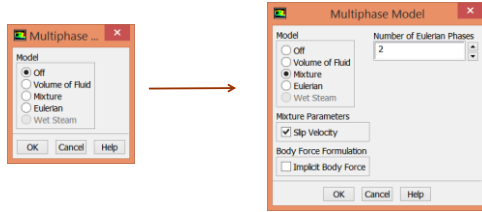


Multiphase models

Volume of Fluid (VOF) Multiphase Model

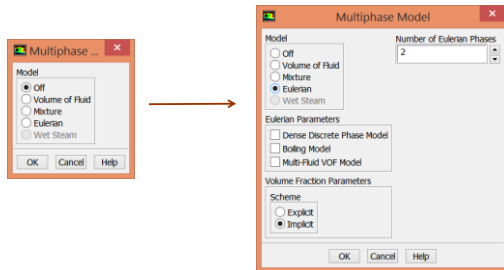


Mixture Multiphase Model

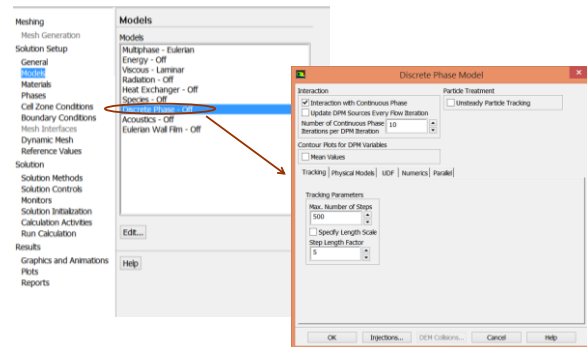


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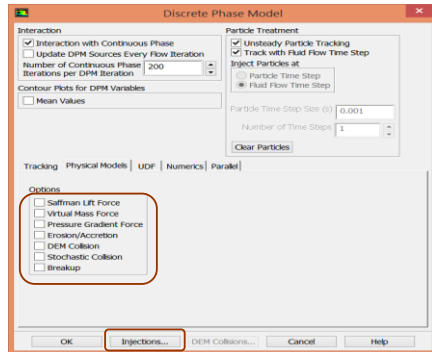
Eulerian Multiphase Model



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- FLUENT contains four distinct multiphase modeling approaches:
 - Volume of Fluid Model (VOF)
 - Eulerian Model
 - Mixture Model
 - Discrete Phase Model (DPM)
- It is important to select the most appropriate solution method 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.

$$St = \frac{\text{Disperse phase time scale}}{\text{Continuous phase time scale}} = \frac{\tau_d}{\tau_c}$$

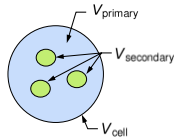
$$\text{where } \tau_c = \frac{D}{U} \text{ and } \tau_d = \frac{\rho_d d_d}{18\mu_c}$$

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- 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.

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

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Turbulence Modeling in Multiphase Flows

- Turbulence modeling with multiphase flows is challenging.
- Presently, single-phase turbulence models (such as $k-\epsilon$ 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.

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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.

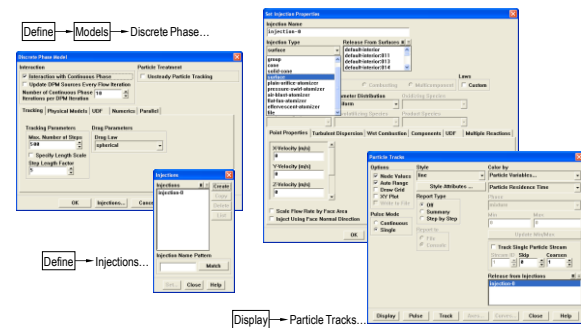
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Discrete Phase Model (DPM) Overview

- 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

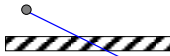
– Flow regime:	Bubbly flow, droplet flow, particle-laden flow
– Volume loading:	Must be dilute (volume fraction $< 12\%$)
– Particulate Loading:	Low to moderate
– Stokes Number:	All ranges of Stokes number
- Application examples
 - Cyclones
 - Spray dryers
 - Particle separation and classification
 - Aerosol dispersion
 - Liquid fuel
 - Coal combustion

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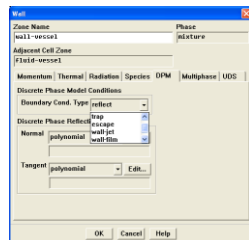
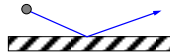
• Escape



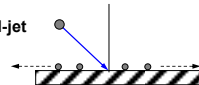
• Trap



• Reflect



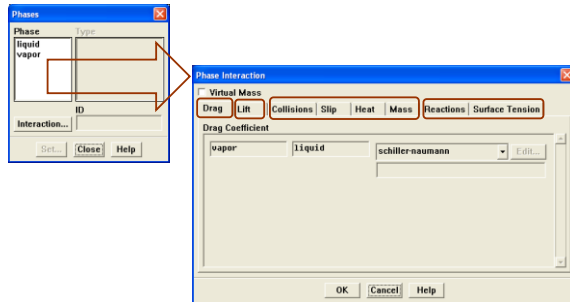
• Wall-jet



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- 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

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- **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:**

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

Solids pressure term is included for granular model.

- The inter-phase exchange forces are expressed as:

In general: $\mathbf{F}_{pq} = -\mathbf{F}_{qp}$ $\mathbf{R}_{pq} = K_{pq}(\mathbf{u}_p - \mathbf{u}_q)$

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

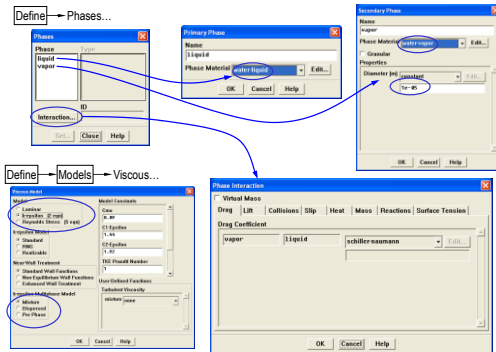
- **Multiphase species transport for species i belonging to mixture of q^{th} phase**

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

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

- 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



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- 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: $St \ll 1$
- Application examples
 - Hydrocyclones
 - Bubble column reactors
 - Solid suspensions
 - Gas sparging

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- 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

$$\frac{\partial \beta_k}{\partial t} + \nabla \cdot (\beta_k \mathbf{u}_k) = -\nabla \cdot (\beta_k \mathbf{u}_k^d)$$

Drift velocity
 $\mathbf{u}_k^d = \mathbf{u}_k - \mathbf{u}_m$

- Solves one equation for the momentum of the mixture

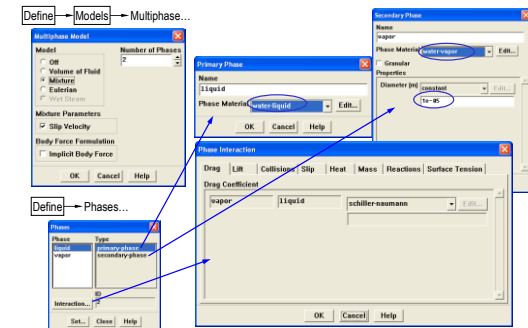
$$\frac{\partial \rho_m \mathbf{u}_m}{\partial t} + \nabla \cdot (\rho_m \mathbf{u}_m \mathbf{u}_m) = -\nabla p + \nabla \cdot [\mu_m (\nabla \mathbf{u}_m + \nabla \mathbf{u}_m^T)] + \rho_m \mathbf{g} + \sum_{k=1}^n \beta_k \rho_k \mathbf{u}_k^d \mathbf{u}_k^d$$

- The mixture properties are defined as:

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

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Advanced Physics Mixture Model Setup

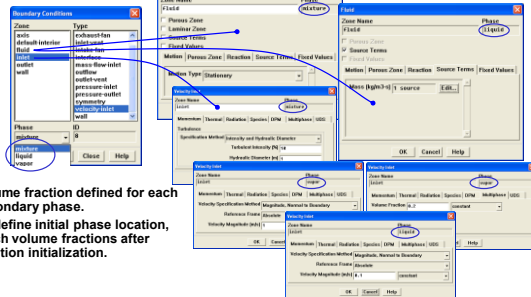


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Advanced Physics Mixture Model Setup



Boundary Conditions



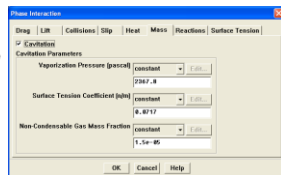
- Volume fraction defined for each secondary phase.
- To define initial phase location, patch volume fractions after solution initialization.

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Advanced Physics Cavitation Submodel



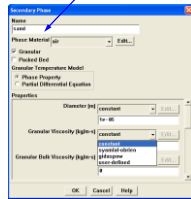
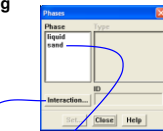
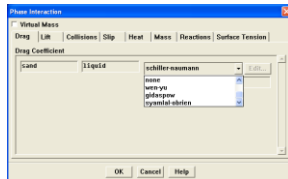
- The Cavitation model models the formation of bubbles when the local liquid pressure is below the vapor pressure.
- The effect of non-condensable gases is included.
- Mass conservation equation for the vapor phase includes vapor generation and condensation terms which depend on the sign of the difference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



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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.



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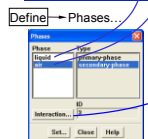
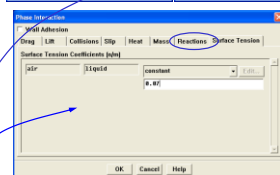
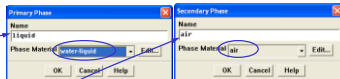
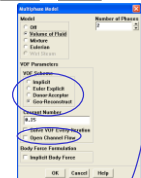
The Volume of Fluid (VOF) Model Overview

- 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

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VOF Model Setup

Define -> Models -> Multiphase...



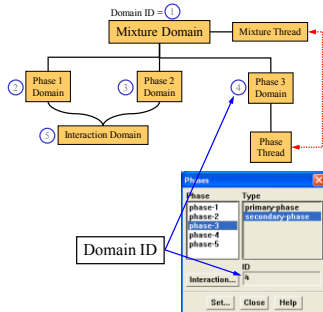
Define -> Operating Conditions...

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

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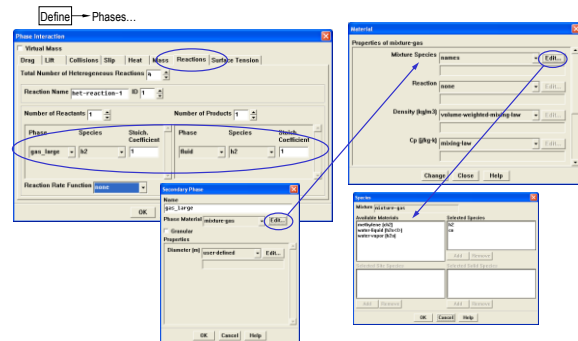
UDFs for Multiphase Applications

- 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.
 - $C_R(\text{cell}, \text{thread})$ 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.



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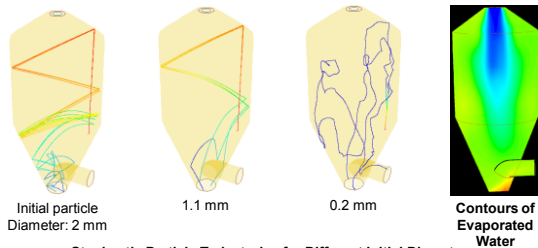
Heterogeneous Reaction Setup



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DPM Example – Spray Drier

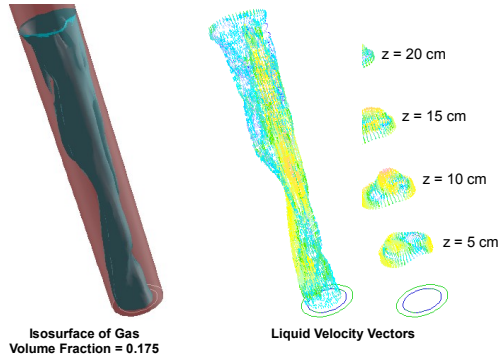
- Spray drying involves the transformation of a liquid spray into dry powder in a heated chamber. The flow, heat, and mass transfer are simulated using the DPM model in FLUENT.



Stochastic Particle Trajectories for Different Initial Diameters

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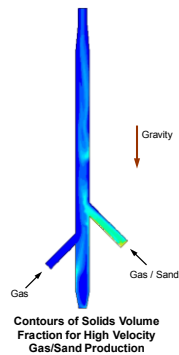
Eulerian Model Example – 3D Bubble Column



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The Granular Option in the Eulerian Model

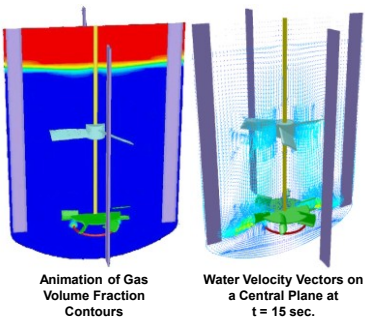
- Granular flows occur when high concentration of solid particles is present. This leads to high frequency of interparticle collisions.
- Particles are assumed to behave similar to a dense cloud of colliding molecules. Molecular cloud theory is applied to the particle phase.
- Application of this theory leads to appearance of additional stresses in 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



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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.

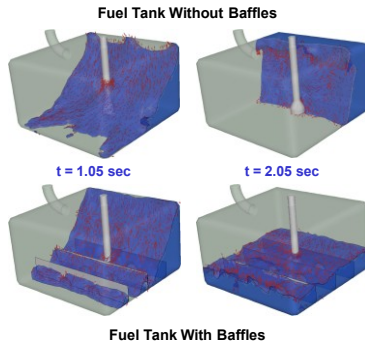


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VOF Example – Automobile Fuel Tank Sloshing

- 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 the tank with internal baffles (at bottom) will keep the fuel intake orifice fully submerged at all times, while the intake orifice is out of the fuel at certain times for the tank without internal baffles (top).



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Reacting Flow Modeling

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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.

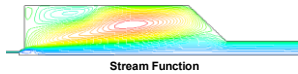
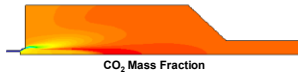
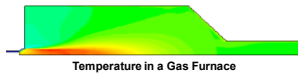
- Within the flow domain, we have already seen how the solver can compute the species concentration and temperature.
- This can then be combined with knowledge of the reaction to form new species in the model, with a corresponding transfer of energy.

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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



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

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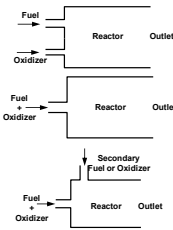
Background

- 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.



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Overview of Reacting Flow Models in FLUENT

FLOW CONFIGURATION

		Premixed	Non-Premixed	Partially Premixed
CHEMISTRY	Fast Chemistry	Eddy Dissipation Model (Species Transport)		
		Premixed Combustion Model	Non-Premixed Equilibrium Model	Partially Premixed Model
		Reaction Progress Variable*	Mixture Fraction	Reaction Progress Variable + Mixture Fraction
	Finite-Rate Chemistry	Laminar Flamelet Model		
		Laminar Finite-Rate Model		
		Eddy-Dissipation Concept (EDC) Model		
		Composition PDF Transport Model		

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

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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.

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Discrete Phase Model (DPM)

- **Description**
 - Trajectories of particles/droplets/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, each with the same initial properties.
 - Interaction among individual particles is neglected.
 - Discrete phase volume fraction must be less than 10%. Mass loading is not limited.
- **Numerous submodels are available.**

$$\frac{d\mathbf{U}_p}{dt} = \mathbf{F}_{drag}(\mathbf{U} - \mathbf{U}_p) + \left(\frac{\rho_p - \rho_f}{\rho_p}\right) \mathbf{g} + \frac{\mathbf{F}}{\rho_p}$$
 - 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.

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Surface Reactions

- **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

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Summary

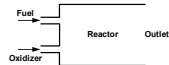
- There are four introductory level tutorials on reacting flow.
 - Species transport and gas combustion
 - Non-premixed combustion
 - Surface chemistry
 - Evaporating liquid spray
- A number of intermediate and advanced tutorials are also available.
- Other learning resources
 - Advanced training course in reacting flow offered by FLUENT
 - User Service Center, www.fluentusers.com
 - All tutorials and lecture notes
 - Web-based training courses

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

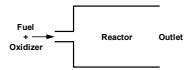
- Applicability
 - Flow Regime: Turbulent flow (high Re)
 - Chemistry: Equilibrium or moderately non-equilibrium (flamelet)
 - Configuration: Non-Premixed only
- Application examples
 - Gas reaction (furnaces, burners). This is usually the model of choice if assumptions are valid for gas phase combustion 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).

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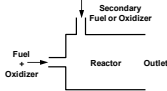
Partially Premixed Combustion Model

• 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.

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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 (NO_x, 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).

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