Computational Fluid Dynamics (CFD) and Multiphase Flow Modelling

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What is CFD?

Computational Fluid Dynamics (CFD) is the science of predicting:
- Fluid flow
- Heat and mass transfer
- Chemical reactions and related phenomena by solving numerically the set of governing mathematical equations.

Conservation of mass, momentum, energy, species, etc.

The results of CFD analyses are relevant in:
- Conceptual studies of new designs
- Detailed product development
- Troubleshooting
- Redesign

CFD analysis complements testing and experimentation
- Reduces the total effort required in the experiment design and data acquisition

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How Does CFD Work?

FLUENT solvers are based on the finite volume method

- Domain is discretized onto a finite set of control volumes (or cells).
- General conservation (transport) equations for mass, momentum, energy, species, etc. are solved on this set of control volumes.

\[
\frac{\partial}{\partial t} \int \rho \psi dV + \int \rho \psi \nabla \cdot \mathbf{V} dA = \int \Gamma \nabla \psi \cdot dA + \int S_\psi dV
\]

- Partial differential equations are discretized into a system of algebraic equations
- All algebraic equations are then solved numerically to render the solution field

<table>
<thead>
<tr>
<th>Equation</th>
<th>Variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>Continuity</td>
<td>1</td>
</tr>
<tr>
<td>X momentum</td>
<td>u</td>
</tr>
<tr>
<td>Y momentum</td>
<td>v</td>
</tr>
<tr>
<td>Z momentum</td>
<td>w</td>
</tr>
<tr>
<td>Energy</td>
<td>h</td>
</tr>
</tbody>
</table>

What is Turbulence?

- Unsteady, irregular motion in which transported quantities (mass, momentum, scalar species) fluctuate in time and space

- Contains a wide range of turbulent eddy sizes (scales spectrum)

- Fluid properties and velocity exhibit random variations
  - Statistical averaging results in accountable, turbulence related transport mechanisms
  - This characteristic allows for turbulence modeling
Overview

Multiphase and multiple component flows are commonly encountered in various fields such as fluid dynamics, environmental science, and engineering. These flows involve the interaction of different phases of matter, such as liquid and gas, or solid and liquid.

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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 gaseous states of matter but can also refer to other forms:
  - Materials with different chemical properties but in the same state or phase (i.e. liquid-liquid, such as, oil-water)

- The fluid system is defined by a primary and multiple secondary phases.
  - There may be several secondary phase denoting particles with different sizes.

- In contrast, multi-component flow (species transport) refers to flow that can be characterized by a single velocity and temperature field for all species.

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Choosing a Multiphase Model

In order to select the appropriate model, users must know a priori the characteristics of the flow in terms of the following:

- **Flow regime**
  - Particulate (bubbles, droplets or solid particles in continuous phase)
  - Stratified (fluids separated by interface with length scale comparable to domain length scale)

- **Multiphase turbulence modeling**

- For particulate flow, one can estimate:
  - Particulate loading ($\beta$)
  - Stokes number (St)

  \[ \beta = \frac{\alpha_d \rho_d}{\alpha_c \rho_c} \]

  \[ \text{St} = \frac{\tau_d}{\tau_c} \quad \text{Where} \quad \tau_d = \frac{\rho_d d_d^2}{18 \mu_c} \quad \text{and} \quad \tau_c = \frac{D}{U} \]

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Multiphase Flow Regimes

- **Gas-Liquid**
  - Bubbly flow – absorbers, evaporators, sparging devices
  - Droplet flow – atomizers, combustors
  - Slug flow – offshore pipe lines
  - Stratified flow – free-surface flow

- **Gas-Solid**
  - Particle – laden flow – cyclone separators, air classifiers, dust collectors, dust-laden environmental flows
  - Fluidized beds – Fluidized bed reactors

- **Liquid-Solid**
  - Slurry flow – Particle flow in liquids, solids suspension, sedimentation, and hydrotransport

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Multiphase Flow Models

"No universal multiphase model for all regimes"

- Volume of Fluid model (VOF)
  Direct method of predicting interface shape between immiscible phases
  Stratified Flow

- Eulerian Model
  Model resulting from averaging of VOF model applicable to dispersed flows
  Dispersed flow

- Mixture Model
  Simplification of Euler model; applicable when inertia of dispersed phase is small
  Dilute Flow

- Lagrangian Dispersed Phase Model (DPM)
  Lagrangian particle/bubble/droplet tracking

The Volume of Fluid Model (VOF)
The Volume of Fluid (VOF) Model

- The VOF model is designed to track the position of the interface between two or more immiscible fluids.
- Tracking is accomplished by solution of phase continuity equation – resulting volume fraction abrupt change points out the interface location.
- A mixture fluid momentum equation is solved using mixture material properties. Thus the mixture fluid material properties experience jump across the interface.
- Turbulence and energy equations are also solved for mixture fluid.
- Surface tension and wall adhesion effects can be taken into account. Phases can be compressible and be mixtures of species.

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Applicability of VOF model

- 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
  - Filling
  - Offshore separator sloshing
  - Boiling
  - Coating

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Summary - VOF

- VOF is an Eulerian fixed-grid technique
- VOF is numerically robust and accurate
- Available in conjunction with most other FLUENT models

Not available with the following reacting flow models:
- Eddy dissipation concept
- Premixed, non-premixed, partially premixed
- Composition PDF
- NOx and soot

The Eulerian Multiphase Model

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The Eulerian Multiphase Model

- The Eulerian multiphase model is a result of averaging of NS equations over the volume including arbitrary particles + continuous phase

- The result is a set of conservation equations for each phase (continuous phase + N particle "media")

- Both phases coexist simultaneously: conservation equations for each phase contain single-phase terms (pressure gradient, thermal conduction etc.) + interfacial terms

- Interfacial terms express interfacial momentum (drag), heat and mass exchange. These are nonlinearly proportional to degree of mechanical (velocity difference between phases), thermal (temperature difference). Hence equations are harder to converge

- Add-on models (turbulence etc.) are available

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Applicability of Eulerian model

- Flow regime - Bubbly flow, droplet flow, slurry flow, fluidized beds, particle-laden flow
- Volume loading - Dilute to dense
- Particulate loading - Low to high
- Turbulence modeling - Weak to strong coupling between phases
- Stokes number - All ranges

- Application examples
  - Fluidized beds
  - High particle loading flows
  - Slurry flows
  - Sedimentation
  - Hydrotransport
  - Risers
  - Packed bed reactors

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Summary – Eulerian model

- Euler model is a powerful tool to model dispersed flows
- Accuracy is determined by accuracy of interfacial terms
- The interfacial terms are usually nonlinear so convergence is often difficult
  - Try solving the case using the unsteady solver
  - Be careful with your choice of particle diameter

Boundary conditions
- Remember that VOF and physical velocity are meaningless. Rather, their roduct (superficial velocity) is related to volume flow rate (i.e. reality).
- Backflow volume fraction of phases is important.

The Mixture Model

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The Mixture Model

- The mixture model is a simplified Eulerian approach for modeling n-phase flows.
- The simplification is based on the assumption that the Stokes number is small (particle and primary fluid velocity is nearly equal in both magnitude and direction).
- Solves the mixture momentum equation (for mass-averaged mixture velocity) and prescribes relative velocities to describe the dispersed phases.
  - Interphase exchange terms depend on relative (slip) velocities which are algebraically determined based on the assumption that St << 1. This means that phase separation cannot be modeled using the mixture model.
  - Turbulence and energy equations are also solved for the mixture if required.
- Solves a volume fraction transport equation for each secondary phase.
- A submodel for cavitation is available.

Applicability of Mixture model

- Flow regime - Bubbly, droplet, and slurry flows
- Volume loading - Dilute to moderately dense
- Particulate Loading - Low to moderate
- Turbulence modeling - Weak coupling between phases
- Stokes Number - St << 1

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

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Summary - Mixture model

- Simple approach
- Easy to use
- Applicable to many multiphase flow problems
- Consider restrictions

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Discrete Phase Model (DPM)

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Discrete Phase Model (DPM)

- 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 of the same initial properties
  - Particle-particle interactions are neglected
  - Turbulent dispersion can be modeled using either stochastic tracking or a "particle cloud" model

- Numerous sub-modeling capabilities 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

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
- Turbulence modeling - Weak to strong coupling between phases
- Stokes Number - All ranges of Stokes number

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

CFD Modelling of Multiphase Flow Systems

- Choose an appropriate model for your application based on flow regime, volume loading, particulate loading, turbulence, and Stokes number
  - Use VOF for free surface and stratified flows
  - Use the Eulerian granular model for high particle loading flows
  - Consider the Stokes number in low to moderate particle loading flows
    - For St > 1, the mixture model is not applicable. Instead, use either DPM or Eulerian
    - For St ≤ 1, all models are applicable. Use the least CPU demanding model based on other requirements

- Strong coupling among phase equations solve better with reduced under-relaxation factors
- Users should understand the limitations and applicability of each model

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Thank you....