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MULTI-PHASE FLOWS
CHARACTERIZATION AND NUMERICAL MODELING

Ing. Paola Ranut, PhD
Prof. Enrico Nobile
pranut@units.it

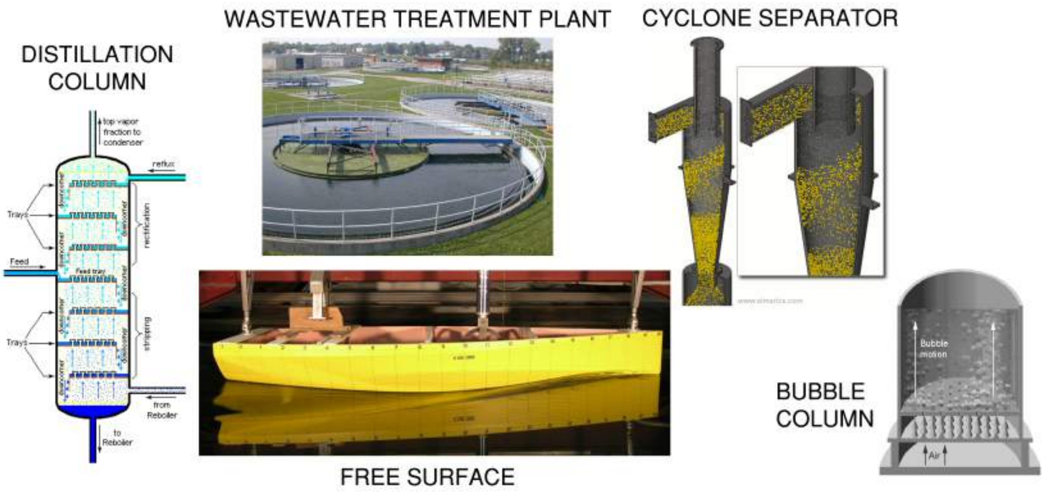
UNIVERSITY OF TRIESTE
DEPARTMENT OF ENGINEERING AND ARCHITECTURE

Outline

CHARACTERIZATION

DEFINITION

- Flow system in which two or more distinct phases flow simultaneously, having some level of phase separation at a scale well above the molecular level;
- Not to be confused with a multicomponent flow (mixture of chemical species, mixed at the molecular level).



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- Not to be confused with a multicomponent flow (mixture of chemical species, mixed at the molecular level).

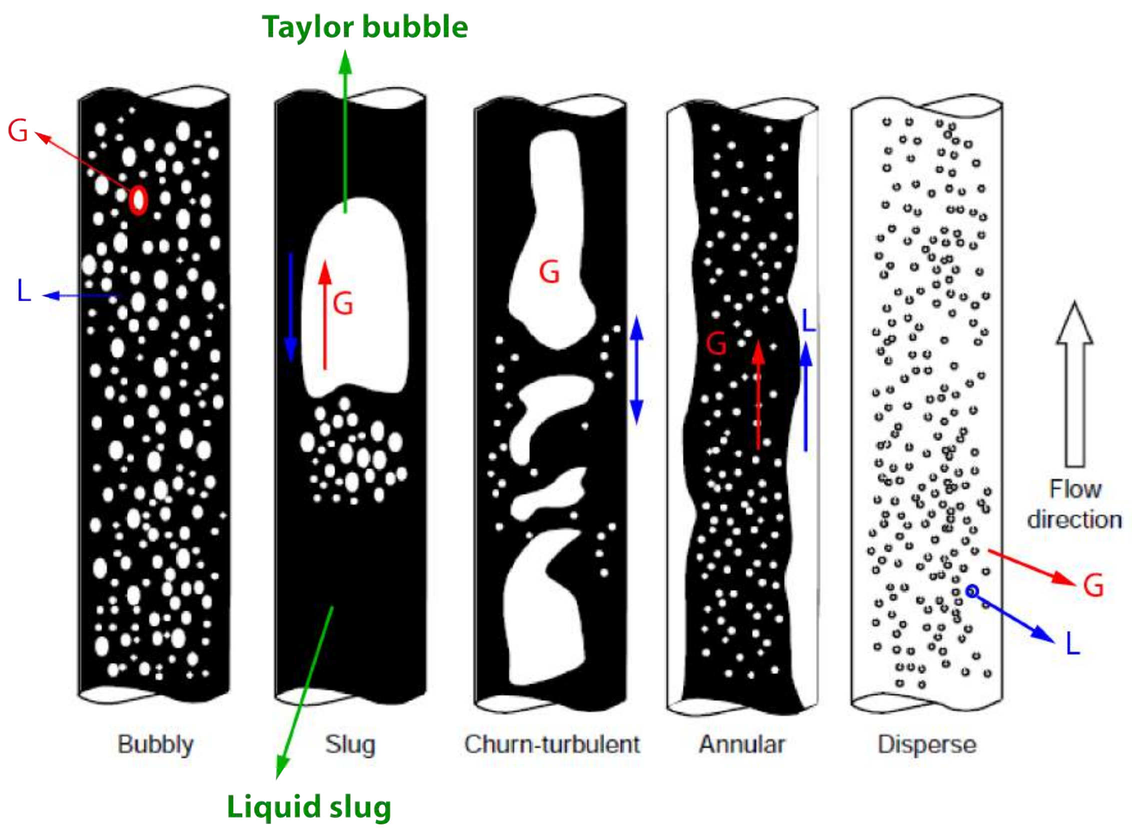
CLASSIFICATION: COMBINATION OF PHASES

- gas-solid flows (dense, dilute, very-dilute)
- liquid-solid flows
- gas-liquid flows $\longrightarrow$ most complex (deformable interface)
- immiscible-liquid mixture (not a real multiphase flow)

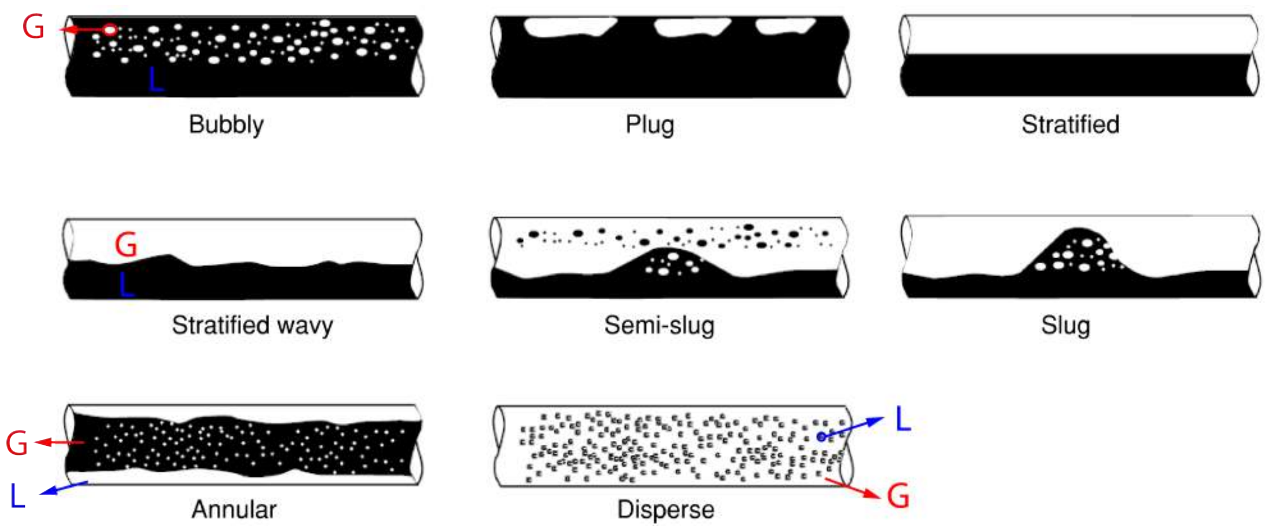
CLASSIFICATION: GEOMETRY OF THE INTERFACE

- disperse flows $\longrightarrow$ gas-solid / liquid-solid flows
- separated flows $\longleftrightarrow$ interfaces
  - fully separated
  - annular (partially separated)
- transitional (mixed) flows

GAS-LIQUID FLOW IN A VERTICAL PIPE



GAS-LIQUID FLOW IN A HORIZONTAL PIPE



FLOW PATTERN MAPS

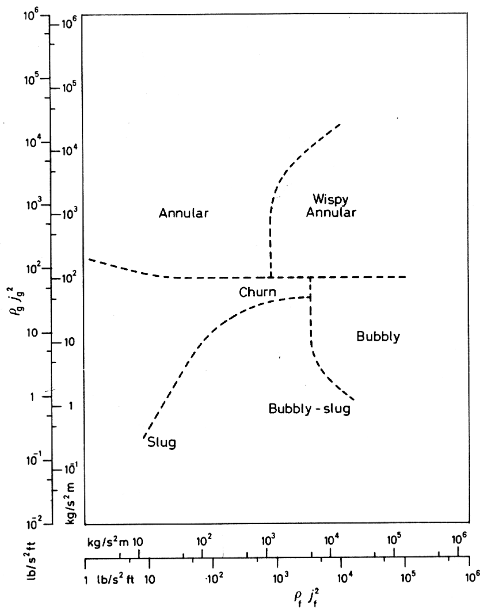


FIGURE: Hewitt and Roberts, two-phase co-current upwards flow in a vertical tube.

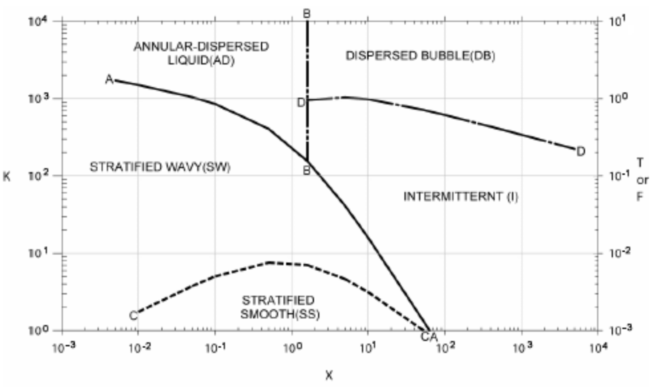


FIGURE: Taitel and Dukler for horizontal co-current flows.

THREE-PHASE FLOWS

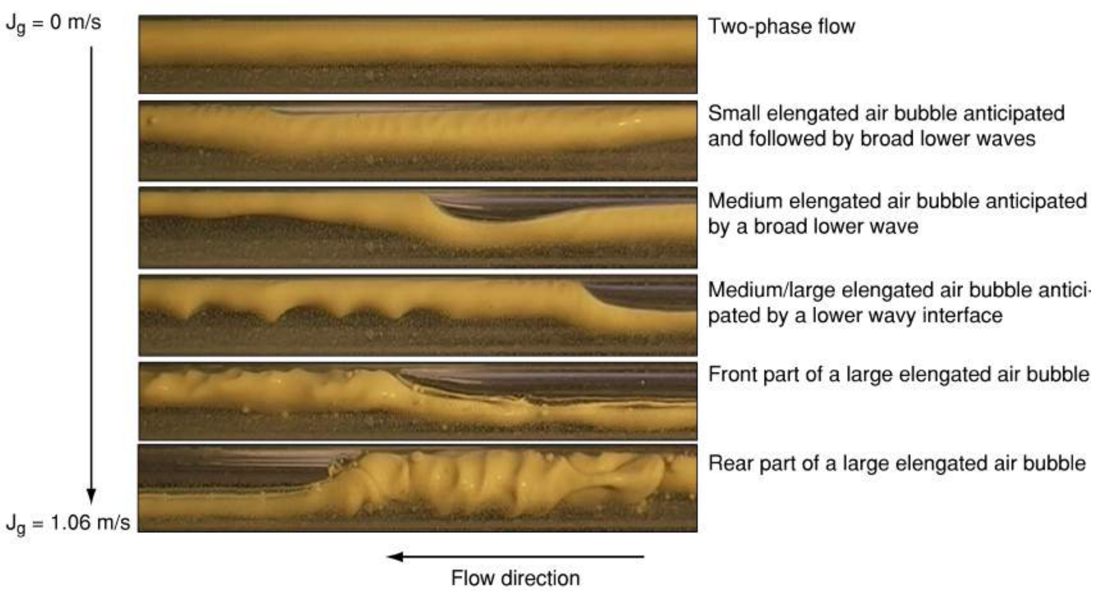


FIGURE: Effect of an increased air input fraction on a three-phase flow, $J_o = 0.46$m/s and $J_w = 0.32$m/s. Photographies taken by the research team of Prof. Sotgia (Politecnico di Milano).

Introduction

- A multiphase flow can be considered as a field subdivided into single-phase regions with moving boundaries separating the constituent phases
- Differential balances hold for each sub-region

Difficulties

- Presence of interfacial surfaces (deformable, in movement)
  - movement is produced by both **convection** and **inter-phase mass transfer**
  - $\Rightarrow$ coupling between field equations of each phase and interfacial conditions
- Discontinuities of properties at interface
  - local jumps in space and time
- Local instant fluctuations (time + space) of the variables (due to motion of interfaces + turbulence)

Introduction

Two stategies

The fluctuation of the variables is space and time allows to follow two different strategies:

- Local instant formulation
  - local instant variables (fluctuations)
  - DNS
  - E.g. evolution of a bubble
- Averaging strategy
  - macroscopic phenomena
  - mean values of fluid motion + properties
  - the local instant description of each phases is replaced by a collective description of the phases
  - the macroscopic properties can be derived by the local instantaneous properties by means of appropriate averaging procedures.

Introduction

Averaging

- Time average

$$\bar{\phi} = \lim_{T\to\infty} \frac{1}{T} \int \phi(x,y,z,t)dt \quad \bar{\phi} = \bar{\phi}(x,y,z) \tag{1}$$

- Space average

$$\langle\phi\rangle_V = \lim_{V\to\infty} \frac{1}{V} \int \phi(x,y,z,t)dt \quad \langle\phi\rangle_V = \langle\phi\rangle\,(t) \tag{2}$$

- Ensemble average

$$\langle\phi\rangle_E = \lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} \phi_n(x,y,z,t)dt \quad \langle\phi\rangle_E = \langle\phi\rangle\,(x,y,z,t) \tag{3}$$

Numerical approaches

Approaches

- *Two-fluid model* $\longrightarrow$ Each phase is considered separately:
  - two sets of averaged conservation equations
  - appropriate conditions at the interface
- *Mixture model* $\longrightarrow$ Mixture modeled as a single fluid with variable properties.
  - 3 conservation equations
  - 1 additional diffusion (continuity) equation ($\leftrightarrow$ concentration changes)

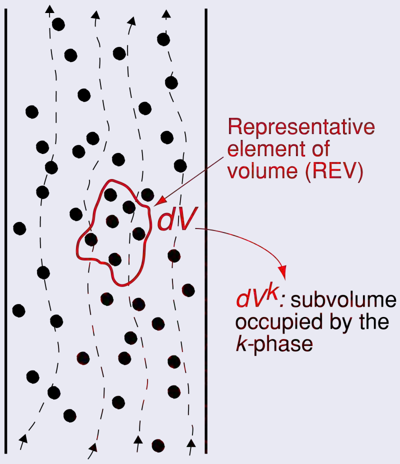
Examples

- Liquid-particle flows
  - Mixture model ($\rho_S \approx \rho_L$)
- Gas-particle flows
  - Two-fluid model (often)
  - Disperse phase: *Eulerian* or *Lagrangian* strategy

Averaging procedure

- At microscopic level: in each subregion or phase, the governing equations are the classical balance laws of continuum mechanics
- In practice, only averaged values of microscopic properties are measured
- Moreover, since the solution of the flow field at the microscale is complex

$\Downarrow$



The system is not described at the micro-scale but a representative volume REV is chosen

$\Downarrow$

Microscopic quantities are averaged on the REV

$\Downarrow$

Local volume averaging

Two-fluid model: foundamentals

Basically, a **phase indicator function** is introduced in the constitutional equations, χ^k

$$\chi^k(\mathbf{x},t) = \begin{cases} 1, & \text{if } \mathbf{x} \text{ is in } k\text{-th phase at time } t, \\ 0, & \text{otherwise} \end{cases} \tag{4}$$

$$\nabla\chi^k = \mathbf{n}^k \delta(\mathbf{x} - \mathbf{x}^{int}, t) \tag{5}$$

$\nabla\chi^k$ is a *generalized function*[a] and behaves like a Dirac δ function.

$\Rightarrow$ $\nabla\chi^k \neq 0$ only at the interface

$\Rightarrow$ χ^k is introduced for convenience, thus to handle some quantities appearing only at the interface.

$$\sum_{k=1}^{M} \chi^k = 1 \qquad \frac{D\chi^k}{Dt} = \frac{\partial \chi^k}{\partial t} + \mathbf{U}^{int} \cdot \nabla\chi^k = 0$$

[a] A generalized function allows to express in a mathematically-corrected form some idealized concepts, as the density of a point or the intensity of an instantaneous source. This reflects the fact that, in reality, a physical quantity cannot be measured at a point but only its mean values can be measured, over sufficiently small neighbourhoods of the given point.

Two-fluid model: foundamentals

Moreover, χ^k is useful for defining

- the volume dV^k of the REV dV occupied by the k-phase:

$$dV^k = \int_{dV} \chi^k dV$$

- the integral of a function f over dV^k

$$\int_{dV^k} f dV^k = \int_{dV} f \chi^k dV$$

The above properties are useful for defining two average operators:

- volume average operator

$$\langle f \rangle = \frac{1}{dV} \int_{dV} f \chi^k dV$$

- mass average operator

$$\bar{f} = \frac{\int_{dV} \rho f \chi^k dV}{\int_{dV} \rho \chi^k dV} = \frac{1}{\langle \rho \rangle \, dV} \int_{dV} \rho f \chi^k dV$$

Two-fluid model: Conservation of mass

Conservation of Mass

$$\frac{\partial \rho^k}{\partial t} + \nabla \cdot (\rho^k \mathbf{U}^k) = 0 \tag{6}$$

By multiplying continuity eq. by χ^k + considering $\frac{\partial \chi^k}{\partial t} + \mathbf{U}^{int} \cdot \nabla \chi^k = 0$

$$\Downarrow$$

Local instant formulation:

$$\frac{\partial (\chi^k \rho^k)}{\partial t} + \nabla \cdot (\chi^k \rho^k \mathbf{U}^k) = \rho^k \left(\mathbf{U}^k - \mathbf{U}^{int} \right) \cdot \nabla \chi^k \tag{7}$$

Instantaneous averaged equation (volume or ensemble averaging):

$$\left\langle \frac{\partial (\chi^k \rho^k)}{\partial t} \right\rangle + \left\langle \nabla \cdot (\chi^k \rho^k \mathbf{U}^k) \right\rangle = \left\langle \rho^k \left(\mathbf{U}^k - \mathbf{U}^{int} \right) \cdot \nabla \chi^k \right\rangle$$

$$\Rightarrow \frac{\partial \left\langle \chi^k \rho^k \right\rangle}{\partial t} + \nabla \cdot \left\langle \chi^k \rho^k \mathbf{U}^k \right\rangle = \boxed{\left\langle \rho^k \left(\mathbf{U}^k - \mathbf{U}^{int} \right) \cdot \nabla \chi^k \right\rangle} \tag{8}$$

$= \Gamma^k$ Interfacial Mass Source

Mass transfer towards the k phase at the interface

$$\sum_{k=1}^{M} \Gamma^k = 0$$

Two-fluid model: Conservation of momentum

Conservation of Momentum

$$\rho^k \frac{\partial \mathbf{U}^k}{\partial t} + \rho^k \mathbf{U}^k \cdot \nabla \mathbf{U}^k = -\nabla p^k + \nabla \cdot \tau^k + \sum \mathbf{F}^{k,\, body\ forces} \tag{9}$$

Instantaneous averaged equation:

$$\begin{aligned} \frac{\partial \left\langle \chi^k \rho^k \mathbf{U}^k \right\rangle}{\partial t} + \nabla \cdot \left\langle \chi^k \rho^k \mathbf{U}^k \otimes \mathbf{U}^k \right\rangle = & \\ & - \nabla \left\langle \chi^k p^k \right\rangle \\ & + \nabla \cdot \left\langle \chi^k \tau^k \right\rangle \\ & + \left\langle \chi^k \right\rangle \left\langle \sum \mathbf{F}^{k,\, body\ forces} \right\rangle \\ & + \left\langle \rho^k \mathbf{U}^k \left(\mathbf{U}^k - \mathbf{U}^{int} \right) \cdot \nabla \chi^k \right\rangle \quad (\leftrightarrow \text{ due to mass exchange}) \\ & + \left\langle \rho^k \right\rangle \left\langle \nabla \chi^k \right\rangle - \left\langle \tau^{\mathbf{k}} \cdot \nabla \chi^k \right\rangle \quad (= \text{Interface Force Density}) \end{aligned} \tag{10}$$

$= \Omega^k$ Interfacial Momentum Source

$$\sum_{k=1}^{M} \Omega^k = F_\sigma$$

Two-fluid model: Conservation of Energy

Conservation of Energy

$$\rho^k \frac{\partial H^k}{\partial t} + \rho^k \mathbf{U}^k \cdot \nabla H^k = -\frac{\partial p^k}{\partial t} - \nabla \cdot \mathbf{q}^k + \sum \mathbf{F}^{k,\, body\ forces} \cdot \mathbf{U}^k + \boxed{\Phi_H^k} \tag{11}$$

$$\Phi_H^k = \nabla \cdot \left(\mathbf{U}^k \cdot \tau^k \right)$$

Viscous term

Instantaneous averaged equation:

$$\begin{aligned} \frac{\partial \left\langle \chi^k \rho^k H^k \right\rangle}{\partial t} + \nabla \cdot \left\langle \chi^k \rho^k \mathbf{U}^k H^k \right\rangle = & \\ & - \frac{\partial \left\langle \chi^k p^k \right\rangle}{\partial t} - \nabla \cdot \left\langle \chi^k \mathbf{q}^k \right\rangle \\ & + \left\langle \chi^k \right\rangle \left\langle \sum \mathbf{F}^{k,\, body\ forces} \cdot \mathbf{U}^k \right\rangle + \boxed{\left\langle \Phi_H'^k \right\rangle} \\ & + \left\langle \rho^k H^k \left(\mathbf{U}^k - \mathbf{U}^{int} \right) \cdot \nabla \chi^k \right\rangle + \left\langle \mathbf{q}^k \nabla \chi^k \right\rangle + \left\langle p^k \right\rangle \left\langle \frac{\partial \chi^k}{\partial t} \right\rangle + \boxed{\left\langle \Phi^{extra} \right\rangle} \end{aligned} \tag{12}$$

$= \Pi_H^k$ Interfacial Energy Source

Two-fluid model: Conservation Equations

Summary: instantaneous averaged equations

$$\frac{\partial\left\langle \chi^k \rho^k \right\rangle}{\partial t} + \nabla \cdot \left\langle \chi^k \rho^k \mathbf{U}^k \right\rangle = \Gamma^k \tag{13}$$

$$\frac{\partial\left\langle \chi^k \rho^k \mathbf{U}^k \right\rangle}{\partial t} + \nabla \cdot \left\langle \chi^k \rho^k \mathbf{U}^k \otimes \mathbf{U}^k \right\rangle = -\nabla \left\langle \chi^k p^k \right\rangle + \nabla \cdot \left\langle \chi^k \tau^k \right\rangle + \left\langle \chi^k \right\rangle \left\langle \sum \mathbf{F}^{k,\, body\,forces} \right\rangle + \Omega^k \tag{14}$$

$$\frac{\partial\left\langle \chi^k \rho^k H^k \right\rangle}{\partial t} + \nabla \cdot \left\langle \chi^k \rho^k \mathbf{U}^k H^k \right\rangle = -\frac{\partial\left\langle \chi^k p^k \right\rangle}{\partial t} - \nabla \cdot \left\langle \chi^k \mathbf{q}^k \right\rangle + \left\langle \chi^k \right\rangle \left\langle \sum \mathbf{F}^{k,\, body\,f.} \cdot \mathbf{U}^k \right\rangle + \left\langle \Phi_H^{\prime k} \right\rangle + \Pi_H^k \tag{15}$$

$$\sum_{k=1}^{M} \Gamma^k = 0 \tag{16}$$

$$\sum_{k=1}^{M} \Omega^k \equiv F_\sigma \tag{17}$$

$$\sum_{k=1}^{M} \Pi_H^k \equiv \varsigma = F_\sigma \cdot \upsilon^{int} \tag{18}$$

Two-fluid model: Conservation Equations

The previous averaged conservation equations can not be solved yet:

Local istantaneous

$$\frac{\partial\left\langle \chi^k \rho^k \right\rangle}{\partial t} + \nabla \cdot \boxed{\left\langle \chi^k \rho^k \mathbf{U}^k \right\rangle} = \Gamma^k$$

Instantanuous average field

Averages of products		Equivalent to further averaging in time
$\Downarrow$	$\longleftrightarrow$	$\langle \phi \rangle = \overline{\langle \phi \rangle} + \phi''$
Products of averages		$\overline{\phi''} = \lim_{T \to \infty} \frac{1}{T} \int \phi'' dt = 0$

Before time-averaging, it is useful to introduce the Favre-averaging approach:

Phase-weighted average

$$\overline{\langle \phi \rangle} = \frac{\overline{\langle \chi^k \phi \rangle}}{\overline{\langle \chi^k \rangle}}$$

Mass-weighted average

$$\widetilde{\langle \psi \rangle} = \frac{\overline{\langle \rho^k \phi \rangle}}{\overline{\langle \rho^k \rangle}}$$

Two-fluid model: Conservation Equations

Time averaging

$$\langle\phi\rangle = \overline{\langle\phi\rangle} + \phi'' \qquad / \cdot \left\langle\chi^k\right\rangle$$

$$\left\langle\chi^k\phi\right\rangle = \left\langle\chi^k\right\rangle \overline{\langle\phi\rangle} + \left\langle\chi^k\right\rangle \phi''$$

Time averaging:

$$\overline{\left\langle\chi^k\phi\right\rangle} = \overline{\left\langle\chi^k\right\rangle \overline{\langle\phi\rangle}} + \overline{\left\langle\chi^k\right\rangle \phi''}$$

$$\overline{\left\langle\chi^k\phi\right\rangle} = \overline{\left\langle\chi^k\right\rangle}\, \overline{\langle\phi\rangle} + \overline{\left\langle\chi^k\right\rangle \phi''}$$

By knowing that:

$$\overline{\langle\phi\rangle} = \frac{\overline{\left\langle\chi^k\phi\right\rangle}}{\overline{\left\langle\chi^k\right\rangle}}$$

$$\Downarrow$$

$$\boxed{\overline{\left\langle\chi^k\phi\right\rangle} = \overline{\left\langle\chi^k\right\rangle}\, \overline{\langle\phi\rangle}} \qquad \overline{\left\langle\chi^k\right\rangle \phi''} = 0$$

The same holds for the mass-weighted average:

$$\overline{\left\langle\rho^k\phi\right\rangle} = \overline{\left\langle\rho^k\right\rangle}\, \overline{\langle\phi\rangle} \qquad \overline{\left\langle\rho^k\right\rangle \phi''} = 0$$

Now we are ready to write the volume and time averaged equations.

Characterization Numerical modeling Gas-particle flows Ansys CFX

Two-fluid model: Conservation Equations

Two-fluid model: Effective Conservation Equations

Conservation of Mass:

$$\frac{\partial \overline{\left\langle\chi^k\rho^k\right\rangle}}{\partial t} + \nabla \cdot \overline{\left\langle\chi^k\rho^k\mathbf{U}^k\right\rangle} = \Gamma^k$$

$$\boxed{\begin{aligned} \overline{\left\langle\chi^k\rho^k\right\rangle} &= \overline{\left\langle\chi^k\right\rangle}\,\overline{\left\langle\rho^k\right\rangle} \\ \overline{\left\langle\chi^k\rho^k\mathbf{U}^k\right\rangle} &= \overline{\left\langle\chi^k\right\rangle}\,\overline{\left\langle\rho^k\mathbf{U}^k\right\rangle} = \overline{\left\langle\chi^k\right\rangle}\,\overline{\left\langle\rho^k\right\rangle}\,\overline{\left\langle\mathbf{U}^k\right\rangle} \end{aligned}}$$

A new quantity can be introduced, that is the *local volume fraction* (or *local concentration*):

$$\alpha^k = \frac{V_k}{V} = \overline{\left\langle\chi^k\right\rangle} \qquad \chi^k \text{ : phase indicator function} \tag{19}$$

By dropping bars and parentheses:

$$\frac{\partial(\alpha^k\rho^k)}{\partial t} + \nabla \cdot (\alpha^k\rho^k\mathbf{U}^k) = \Gamma'^k \tag{20}$$

TWO-FLUID MODEL: CONSERVATION EQUATIONS

TWO-FLUID MODEL: EFFECTIVE CONSERVATION EQUATIONS

$$\alpha^k = \frac{V_k}{V} = \left\langle \chi^k \right\rangle \qquad \chi^k \text{ : phase indicator function}$$

Conservation of Mass:

$$\frac{\partial(\alpha^k \rho^k)}{\partial t} + \nabla \cdot (\alpha^k \rho^k \mathbf{U}^k) = \Gamma'^k$$

Conservation of Momentum:

$$\frac{\partial(\alpha^k \rho^k \mathbf{U}^k)}{\partial t} + \nabla \cdot (\alpha^k \rho^k \mathbf{U}^k \otimes \mathbf{U}^k) = -\alpha^k \nabla p^k - p^k \nabla \alpha^k + \nabla \cdot (\alpha^k \tau^k) - \nabla \cdot (\alpha^k \tau^{k''}) + \alpha^k \sum \mathbf{F}^{k,\, b.f.} + \Omega'^k \tag{21}$$

Conservation of Energy:

$$\begin{aligned} \frac{\partial(\alpha^k \rho^k H^k)}{\partial t} + \nabla \cdot (\alpha^k \rho^k \mathbf{U}^k H^k) =& p^k \frac{\partial \alpha^k}{\partial t} + \alpha^k \frac{\partial p^k}{\partial t} - \nabla \cdot (\alpha^k \mathbf{q}^k) - \nabla \cdot (\alpha^k \mathbf{q}_H^{k''}) \\ &+ \alpha^k \sum \mathbf{F}^{k,\, body\ forces} \cdot \mathbf{U}^k + \Phi_H^{``k} + \Pi_H'^k \end{aligned} \tag{22}$$

Algebraic constraint on α:

$$\sum_{k=1}^{M} \alpha^k = 1 \tag{23}$$

MIXTURE MODEL

MIXTURE MODEL

The dynamic interaction of the phases in neglected, since the interfacial exchange term are omitted.

The mixture is modeled as a single fluid with variable properties

$$\rho^m = \sum_{k=1}^{2} \alpha^k \rho^k, \quad \mu^m = \sum_{k=1}^{2} \alpha^k \mu^k, \quad \lambda^m = \sum_{k=1}^{2} \alpha^k \lambda^k$$

$$\mathbf{U}^m = \frac{\sum_{k=1}^2 \alpha^k \rho^k \mathbf{U}^k}{\sum_{k=1}^2 \alpha^k \rho^k}, \quad H^m = \frac{\sum_{k=1}^2 \alpha^k \rho^k H^k}{\sum_{k=1}^2 \alpha^k \rho^k}$$

Conservation of Mass:

$$\frac{\partial \rho^m}{\partial t} + \nabla \cdot (\rho^m \mathbf{U}^m) = 0$$

Conservation of Momentum:

$$\begin{aligned} \frac{\partial(\rho^m \mathbf{U}^m)}{\partial t} + \nabla \cdot (\rho^m \mathbf{U}^m \otimes \mathbf{U}^m) =& -\nabla p + \nabla \cdot \left[\mu^m (\nabla \mathbf{U}^m) + (\nabla \mathbf{U}^m) - \frac{2}{3} \mu^m \nabla \cdot \mathbf{U}^m \delta \right] \\ &- \nabla \cdot \tau^{m''} + \rho^m \mathbf{g} + \mathbf{F}_\sigma \\ &- \nabla \cdot \sum_{k=1}^{2} (\alpha^k \rho^k \mathbf{U}^{dr,k} \otimes \boxed{\mathbf{U}^{dr,k}}) \end{aligned}$$

Drift velocity $\mathbf{U}^{dr,k} = \mathbf{U}^k - \mathbf{U}^m$

MIXTURE MODEL

MIXTURE MODEL

Conservation of Mass:

$$\frac{\partial \rho^m}{\partial t} + \nabla \cdot (\rho^m \mathbf{U}^m) = 0 \tag{24}$$

Conservation of Momentum:

$$\begin{aligned}\frac{\partial(\rho^m \mathbf{U}^m)}{\partial t} + \nabla \cdot (\rho^m \mathbf{U}^m \otimes \mathbf{U}^m) = &- \nabla p + \nabla \cdot \left[\mu^m (\nabla \mathbf{U}^m) + (\nabla \mathbf{U}^m) - \frac{2}{3}\mu^m \nabla \cdot \mathbf{U}^m \delta\right] \\ &- \boxed{\nabla \cdot \tau^{m''}} + \rho^m \mathbf{g} + \boxed{\mathbf{F}_\sigma} \\ &- \nabla \cdot \sum_{k=1}^{2} (\alpha^k \rho^k \mathbf{U}^{dr,k} \otimes \boxed{\mathbf{U}^{dr,k}})\end{aligned} \tag{25}$$

Drift velocity $\mathbf{U}^{dr,k} = \mathbf{U}^k - \mathbf{U}^m$

Conservation of Energy:

Turbulent fluxes

$$\frac{\partial(\rho^m H^m)}{\partial t} + \nabla \cdot (\rho^m \mathbf{U}^m H^m) = \nabla \cdot (\lambda^m \nabla T^m) - \boxed{\nabla \cdot \mathbf{q}_H^{m''}} + \boxed{\varsigma} - \nabla \cdot \sum_{k=1}^{2} (\alpha^k \rho^k \mathbf{U}^{dr,k} H^k) \tag{26}$$

Tension effects

Algebraic constraint on α:

$$\sum_{k=1}^{2} \alpha^k = 1 \tag{27}$$

CHARACTERIZATION NUMERICAL MODELING GAS-PARTICLE FLOWS ANSYS CFX

MIXTURE MODEL

HOMOGENEOUS MODEL

- Simplification of the Mixture model valid when the phases move at the same velocity $\Rightarrow \mathbf{U}^{dr,k} = 0$
- It can be used for:
  - finely dispersed flows
  - flows with separated phases (e.g., stratified or wavy flows, free surface flows)

Generic form of the governing equations

Two-fluid model

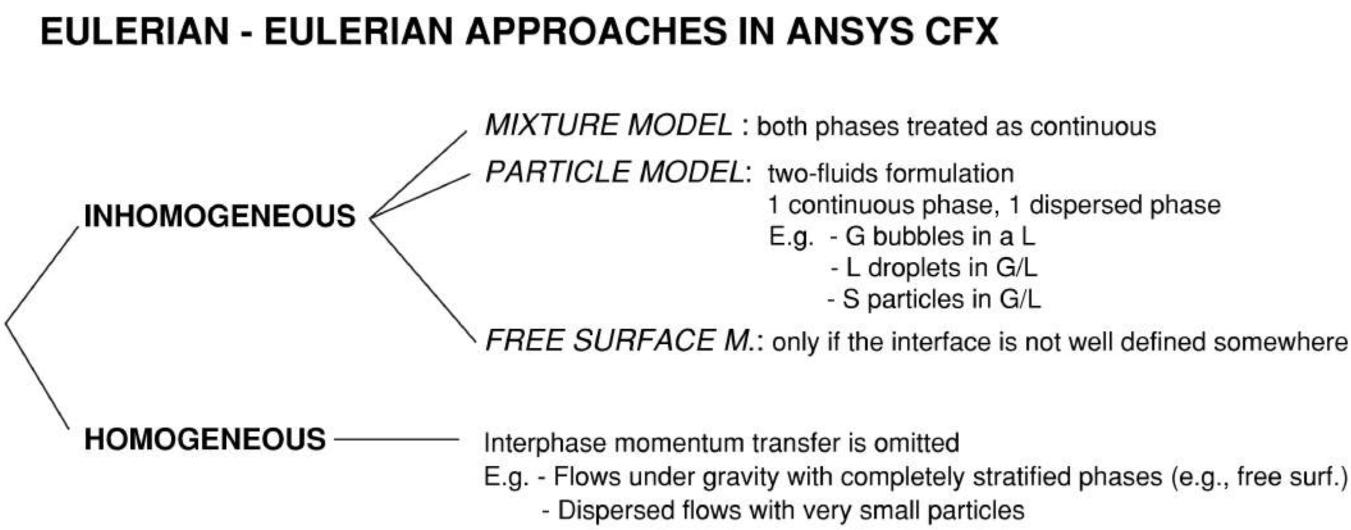
$$\frac{\partial(\alpha^k \rho^k \phi^k)}{\partial t} + \nabla \cdot (\alpha^k \rho^k \mathbf{U}^k \otimes \phi^k) = \nabla \cdot \left[\alpha^k \Gamma^k_{\phi^k} (\nabla \mathbf{U}^k)\right] + S^k_{\phi^k} \quad (28)$$

Mixture model

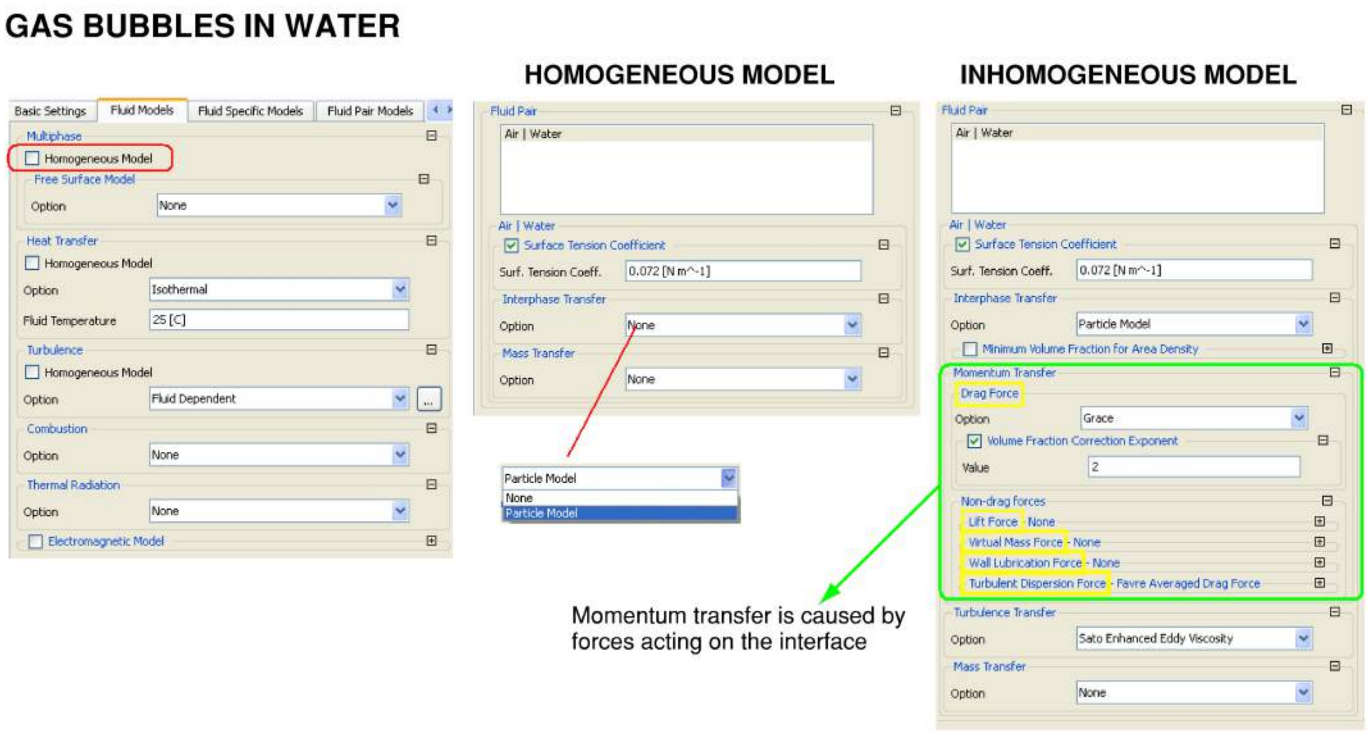
$$\frac{\partial(\rho^m \phi^m)}{\partial t} + \nabla \cdot (\rho^m \mathbf{U}^m \otimes \phi^m) = \nabla \cdot \left[\Gamma_{\phi^m} (\nabla \mathbf{U}^m)\right] + S_{\phi^m} \quad (29)$$

Diffusion coefficiant

ANSYS CFX: Available models



ANSYS CFX: Homogeneous vs Inhomogeneous



Eulerian vs Lagrangian

Two strategies

The continuous phase is always treated in an Eulerian manner.
The discrete particulate can be treated as both a continuous or a discrete phase. Therefore, two different approaches exist:

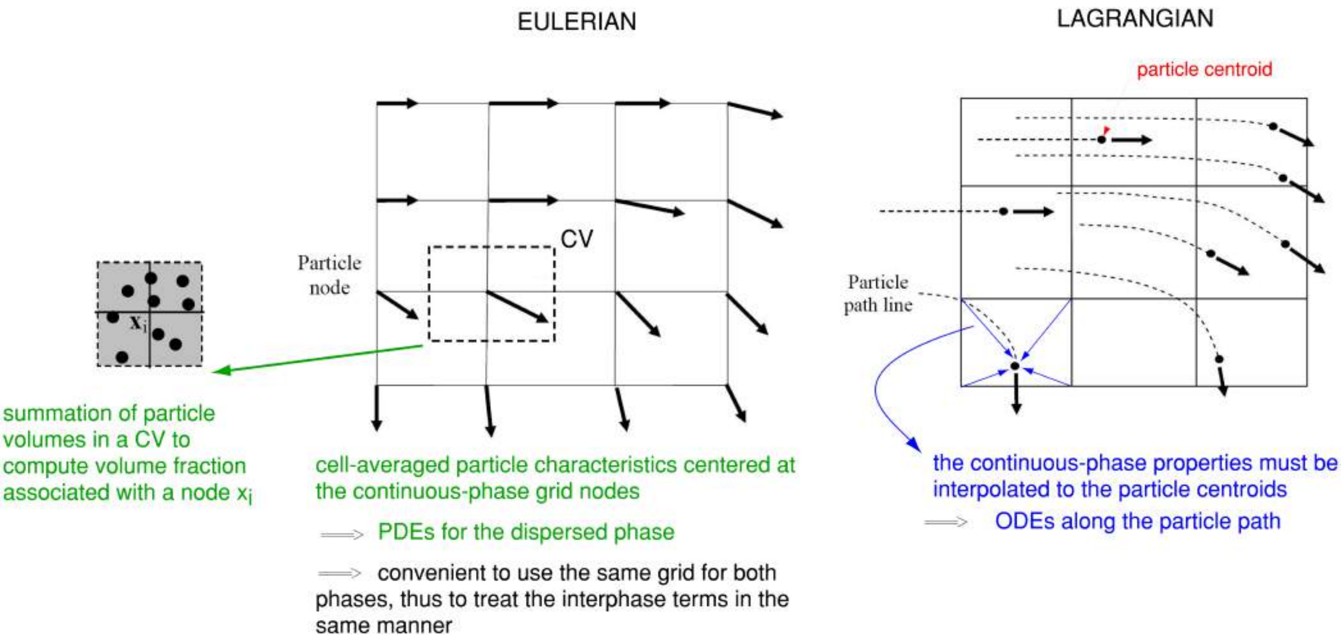
Eulerian - Eulerian

- Particles are regarded as a continuous phase
- Two-fluid model
- *The reference frame is stationary*

Eulerian - Lagrangian

- The motion of individual particles (or of a cloud, *parcel*, of them) is tracked throughout the domain
- *The reference frame moves with the particles*
- Position and velocity of the particle is a function of time only
  - The time average is done by following a certain particle for a chosen time interval
- Forces acting on particles are considered
  - Position and velocity of the particle are computed from Newton's 2nd Law (force balance)
- If the number of particles is large, a statistical approach is adopted.

EULERIAN VS LAGRANGIAN



PHASE COUPLING

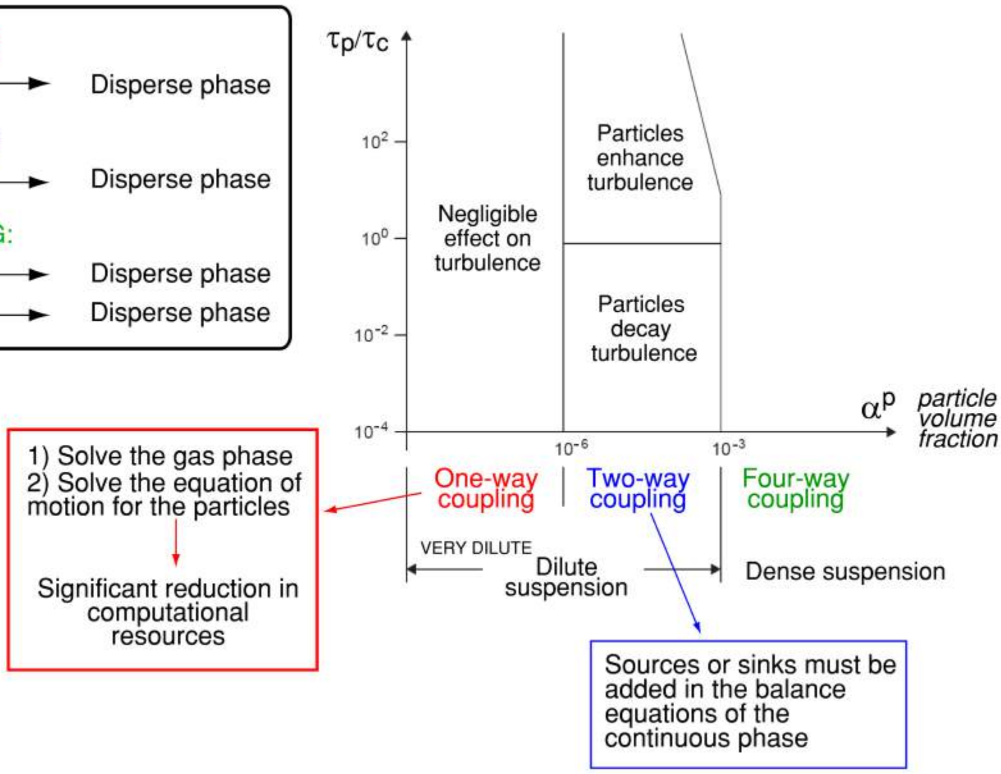
τ_p : *particle relaxation time*

τ_c : *characteristics time of collisions*

ONE-WAY COUPLING:
Continuous phase → Disperse phase

TWO-WAY COUPLING:
Continuous phase ↔ Disperse phase

FOUR-WAY COUPLING:
Continuous phase ↔ Disperse phase
Disperse phase ↔ Disperse phase



PHASE COUPLING AND NUMERICAL STRATEGY

- Polidisperse one-way coupling
  - LAGR: very efficient
  - EULER: computationally intensive ($\longleftrightarrow$ multiple Eulerian particle fields)
- Two-way coupling
  - LAGR: can be one order of magnitude less efficient
  - EULER: numerically convenient (same grid for continuous and disperse phase $\Longrightarrow$ no interpolation errors)
- Four-way coupling
  - LAGR: more accurate
  - EULER / LAGR(parcel): if the number of particles in the system is large ($\geq 10^5$) and/or the collision frequency is high, $\Longrightarrow$ more practical to capture only the mean effects
- Wall interactions
  - LAGR: accurately captured (the distance from the particle centroid to the wall is directly computed)
  - EULER / LAGR(parcel): not efficient (the vast majority of the particles are many particle diameters away from the wall)

EULERIAN-LAGRANGIAN FRAMEWORK

TRAJECTORY EQUATION

$$\underbrace{\rho^p V_p}_{m_p} \frac{D\mathbf{U}^p_{ins}}{Dt} = \underbrace{S_{V^p}}_{\sum \mathbf{F}} \tag{30}$$

Forces acting on the particulate:

- *Drag force*: induced by the surrounding fluid (pressure field + viscous stress);
- *Virtual or added mass force*: difference in acceleration fluid/particulate;
- *Lift force*
- *Body force due to gravity*
- *Bouyancy force*: difference in density between phases; almost always important.
- *Magnus force*: rotating particulate in a non-rotating fluid
- *Pressure gradient force*
- *Basset force*: temporal delay in boundary layer development as the relative velocity changes with time

Eulerian-Lagrangian framework

Trajectory equation (dilute regime)

$$\underbrace{\rho^p V_p}_{m_p} \frac{D\mathbf{U}^p_{ins}}{Dt} = \underbrace{S_{Vp}}_{\sum \mathbf{F}}$$

For dilute regimes $\alpha^p < 10^{-3}$:

$$\frac{D\mathbf{U}^p_{ins}}{Dt} = \frac{1}{\tau_p}\left(\mathbf{U}^g_{ins} - \mathbf{U}^p_{ins}\right) + \left(1 - \frac{\rho^g}{\rho^p}\right)\mathbf{g} \quad (31)$$

Particle response time

$$\mathbf{U}^g_{ins} = \mathbf{U}^g + \boxed{\mathbf{U}''^g} \quad (32)$$

Instant velocity

- The Favre-averaged form of the transport equations for the continuous phase generally yields the mean values
- The key problem in many Lagrangian-tracking models is to adequately estimate the unknown fluctuating component of the fluid velocity at every particulate location, as it travels in discrete time steps through the computational domain.

Eulerian-Lagrangian framework

Trajectory equation (dilute regime)

For $\alpha^p < 10^{-3}$:

$$\frac{D\mathbf{U}^p_{ins}}{Dt} = \frac{1}{\tau_p}\left(\mathbf{U}^g_{ins} - \mathbf{U}^p_{ins}\right) + \left(1 - \frac{\rho^g}{\rho^p}\right)\mathbf{g}$$

$$\mathbf{U}^g_{ins} = \mathbf{U}^g + \boxed{\mathbf{U}''^g}$$

- Omitting $\mathbf{U}''^g$ $\leftrightarrow$ ignoring the particulate dispersion due to turbulent velocity fluctuation

  $\Downarrow$

  Particulates with same physical properties/initial conditions $\Rightarrow$ identical trajectories (*Deterministic models*)

- On the contrary, turbulent fluctuations $\Rightarrow$ different trajectories even for particulates with the same physical properties/initial conditions (*Stochastic models*)
  - when the particulate enters an eddy, the eddy's fluctuating velocity U''^g is added to $\mathbf{U}^g$
  - U''^g is randomly sampled from a Probability Density Function: $U''^g = \varsigma\sqrt{\frac{2}{3}k}$
  - at the end of each time step, a new fluctuating fluid velocity is sampled from a new PDF
- With stochastic models the computational burden increases

Eulerian-Lagrangian framework

Governing equations for the continuous phase (dilute regime)

For dilute regimes $\alpha^p < 10^{-3}$:

Conservation of Mass

$$\frac{\partial \rho^g}{\partial t} + \nabla \cdot (\rho^g \, \mathbf{U}^g) = 0 \tag{33}$$

Conservation of Momentum

$$\frac{\partial \rho^g U_i^g}{\partial t} + \frac{\partial}{\partial x_j}(\rho^g U_j^g U_i^g) = \frac{\partial}{\partial x_j}\left(\mu^g + \mu_T^g\right)\frac{\partial U_i^g}{\partial x_i} + S_{U_i^g} \tag{34}$$

$$S_{U_i^g} = -\frac{\partial p'^g}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\mu^g + \mu_T^g\right)\frac{\partial U_j^g}{\partial x_i} + \boxed{S_{U\,i}^p} \tag{35}$$

p'^g is a modified averaged pressure.

Particles' influence on the gas phase

If $\alpha^p < 10^{-6} \Rightarrow \mathbf{S}_U^p = 0$

ONE WAY coupling

Eulerian-Eulerian framework

Governing Equations

- dilute gas-particle applications
- a set of continuum conservation equations, representing both the gas and particle species, is solved

On the basis of the *two-fluid model*:

Conservation of Mass:

$$\frac{\partial \rho^{bp}}{\partial t} + \nabla \cdot (\rho^{bp} \, \mathbf{U}^p) = 0 \tag{36}$$

Conservation of Momentum:

Gravity Drag

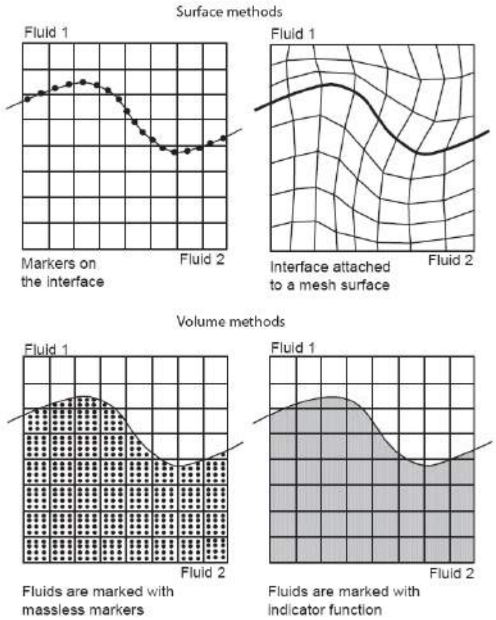
$$\frac{\partial \rho^{bp}\mathbf{U}^{bp}}{\partial t} + \nabla \cdot (\rho^{bp}\mathbf{U}^{bp}\mathbf{U}^p) = \nabla \cdot \tau + \boxed{\mathbf{F}_G} + \boxed{\mathbf{F}_D} + \boxed{\mathbf{F}_{WM}} \tag{37}$$

Particle-wall interaction

For dilute applications:

$$\rho^{bp} = \alpha^p \rho^p = \frac{V_p}{V}\rho^p \qquad \alpha^p : \textit{local volume fraction} \tag{38}$$

INTERFACE CAPTURING METHODS



- **surface methods**: track the interface explicitly:
  - mark the interface with marker points (particles)
  - attach the interface to a mesh surface, which is forced to move ⇒ moving grid
- **volume methods**: both fluids treated as single continuum. The fluids on either side of the interface are marked by either *particles* of negligible mass or an *indicator function*

↓

fixed (Eulerian) grid

  - simple
  - can handle strong topological deformations
  - sometimes, significant increase in memory and time
  - under certain circumstances, fails to calculate accurately the surface tension force at the interface
  - e.g. volume-of-fluid and level-set approaches

VOLUME METHODS: VOLUME OF FLUID

VOLUME OF FLUID

- Fixed grid
- *One-fluid* formulation (*Mixture model*)
- Conservative
- Can not resolve details of the interface < than the mesh size

- The interface is tracked in an indirect way: the volume fraction of a phase is evolved in time
- A scalar indicator function F (*Colour function*) is defined for one particular fluid (liquid), corresponding to the volume fraction :

$$F = \lim_{V\to\infty} \frac{1}{V} \int\int\int \chi^k(x,y,z,t)\, dV = \left\langle \chi^k \right\rangle \tag{39}$$

  - $F = 1$: fluid 1
  - $F = 0$: fluid 2
  - $0 < F < 1$: interface present

VOLUME METHODS: VOLUME OF FLUID

VOLUME OF FLUID

- A *one-fluid* formulation is used:

$$\rho(F) = \rho_l F + \rho_g(1 - F) \tag{40}$$

$$\mu(F) = \mu_l F + \mu_g(1 - F) \tag{41}$$

- An advection equation for the volume fraction F need to be solved

$$\frac{\partial F}{\partial t} + \nabla \cdot (F\mathbf{U}) = 0 \tag{42}$$

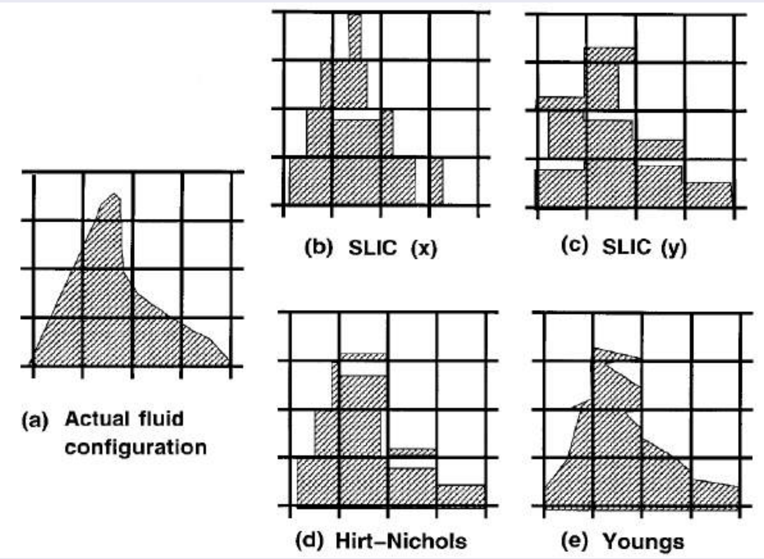
- The VOF algorithm consists of three major parts:
  - *interface reconstruction* method: explicit description of the interface in each cell, based on F at the current time step;
  - *advection algorithm*: computation of the distribution of F at the next time step (Eq. (42)) by using the reconstructed interface and the current velocity field;
  - *surface tension model*: to account for the surface tension effects at the interface.

The success of a VOF method is strongly connected to the numerical scheme used for the advection of the F.

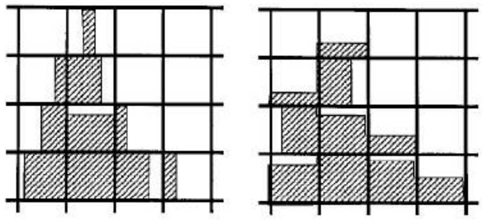
VOLUME METHODS: VOLUME OF FLUID

INTERFACE RECONSTRUCTION

- piecewise constant approximation: SLIC, Donor-acceptor (Hirt and Nichols)
- piecewise linear approximation: PLIC (Young) FLAIR, LVIRA, FLVIRA



Volume methods: Volume of fluid

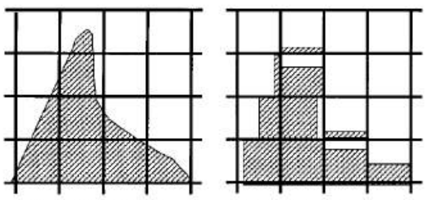


(b) SLIC (x) (c) SLIC (y)

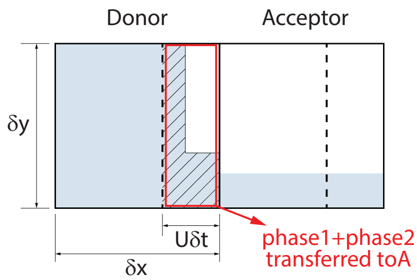
Interface reconstruction

- Sequence of line segments aligned with the grid
- The interface can assume different configurations for each sweep direction (x and y)

Volume methods: Volume of fluid



(a) Actual fluid configuration (d) Hirt–Nichols



Donor-acceptor (Hirt and Nichols)

- Donor: C.V. providing the fluid
- Acceptor: C.V. receiving the fluid
- The amount of F fluxed across the cell face in one time step:

$$\delta F \delta y = \min\left[F_{AD}\left|\mathbf{U}\delta t\right|\delta y + CF,\ F_D \delta x \delta y\right] \tag{43}$$

$$CF = \max\left[(1 - F_{AD})\left|\mathbf{U}\delta t\right|\delta y - (1 - F_D)\delta x \delta y,\ 0\right] \tag{44}$$

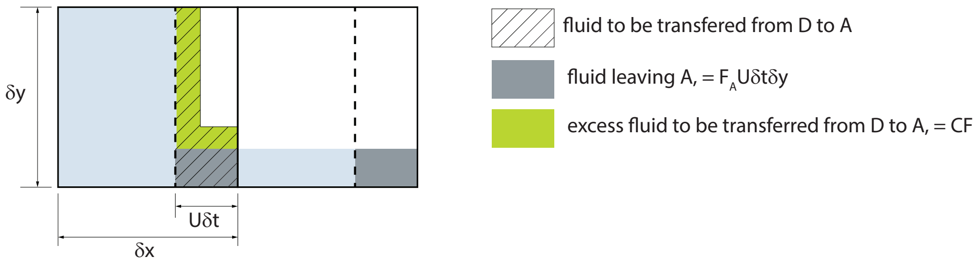
$F_{AD}\ |\mathbf{U}\delta t|\ \delta y + CF$: amount of fluid transferred to the acceptor cell
$F_D\delta x\delta y$: amount of fluid available in the donor cell
$(1 - F_{AD})\ |\mathbf{U}\delta t|$: amount of void to be fluxed to A
$(1 - F_D)\delta x\delta y$: amount of void in the donor cell

Volume methods: Volume of fluid

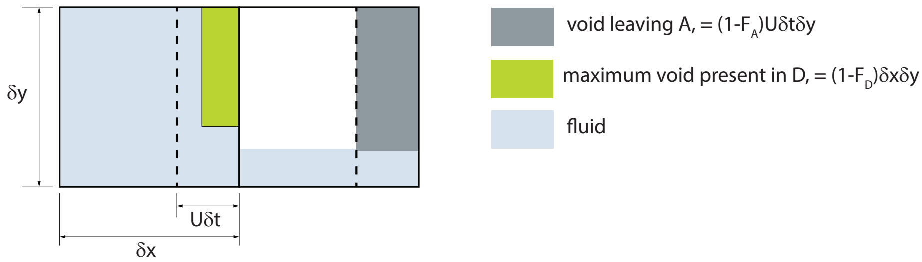
If $F_{AD} = F_A$:

$$\delta F \delta y = \min\left[F_A \left|\mathbf{U}\delta t\right| \delta y + CF,\ F_D \delta x \delta y\right]$$
$$CF = \max\left[(1 - F_A)\left|\mathbf{U}\delta t\right| \delta y - (1 - F_D)\delta x \delta y,\ 0\right]$$

Fluid phase



Void phase



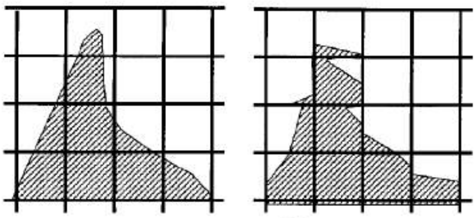
Volume methods: Volume of fluid

Note

$$\delta F \delta y = \min\left[F_{AD} \left|\mathbf{U}\delta t\right| \delta y + CF,\ F_D \delta x \delta y\right]$$
$$CF = \max\left[(1 - F_{AD})\left|\mathbf{U}\delta t\right| \delta y - (1 - F_D)\delta x \delta y,\ 0\right]$$

The Donor-Acceptor VOF method uses first-order upwind and downwind fluxes combined in such a way as to ensure stability of the numerical calculation and at the same time as to minimize diffusion

Volume methods: Volume of fluid



PLIC (Youngs)

- oblique lines: $n^x x + n^y y = \beta$

  1) compute $\vec{n}$
  2) compute β thus to ensure the correct placement of the line

  $\updownarrow$

  The fraction of the cell area cut by the linear segment and occupied by the reference phase must equal F.

- interface is not required to be a continuous chain of segments
- very robust and efficient, but only of first-order accuracy

Volume methods: Level-set method

Level-set method)

- The interface is defined by a level-set function $\phi = \pm d(x,t)$ (signed shortest distance of point x from the interface at time t)
- Transport equation for ϕ

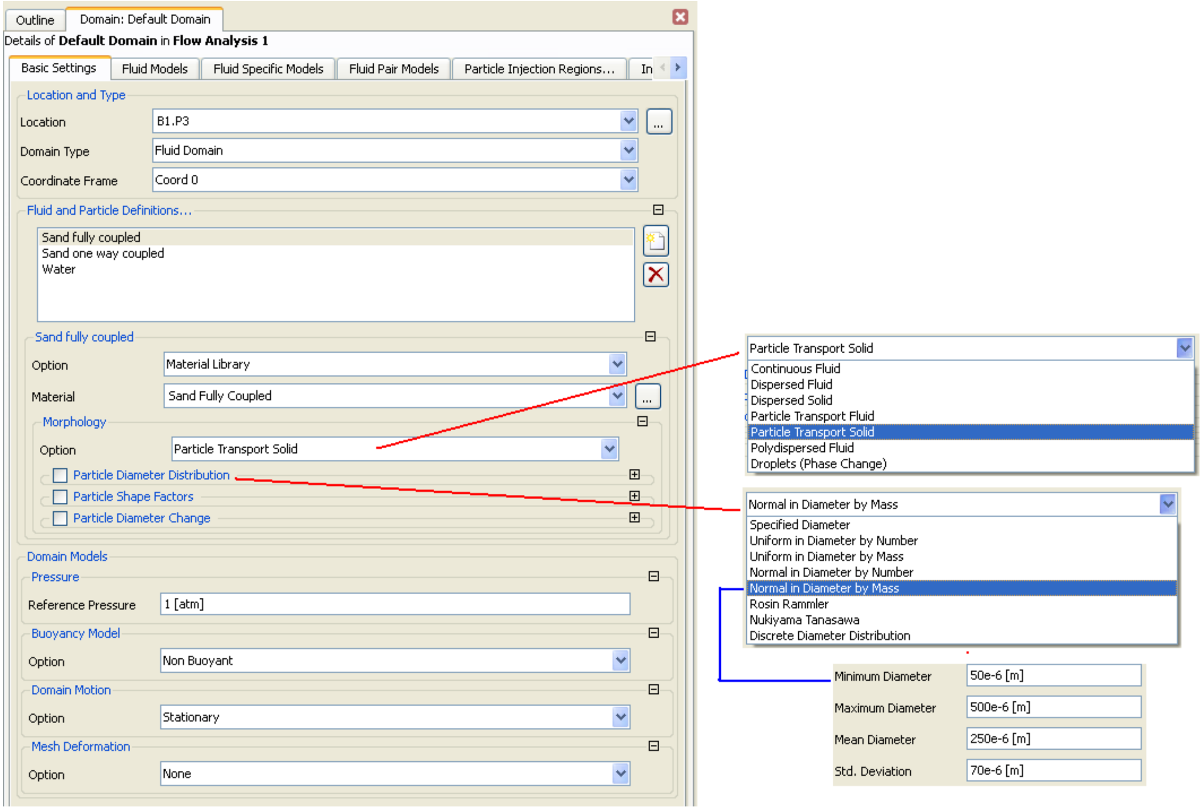
$$\frac{\partial \phi}{\partial t} + \mathbf{U}^m \cdot \nabla \phi = S \tag{45}$$

- The generic fluid property $b(\mathbf{x},t)$ is calculated by interpolating the values of the two phases, b_1 and b_2:

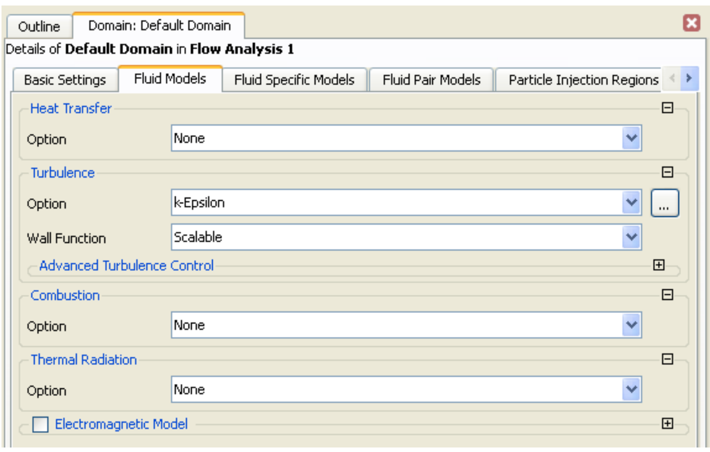
$$b(\mathbf{x},t) = (1 - H_\varepsilon(\phi(\mathbf{x},t)))b_1 + H_\varepsilon(\phi(\mathbf{x},t))b_2 \tag{46}$$

- During the solution of Eq. (45), ϕ may not remain a signed distance function at later times:
  - interface smearing, numerical diffusion and difficulties in preserving the mass conservation
  - re-initialization techniques for ϕ
- For the interpolation of the advective term $\mathbf{U}^m \cdot \nabla \phi$:
  - a non-diffusive scheme must be adopted
  - if the mesh is not sufficiently fine $\Rightarrow$ higher-order schemes $\Rightarrow$ no smearing.

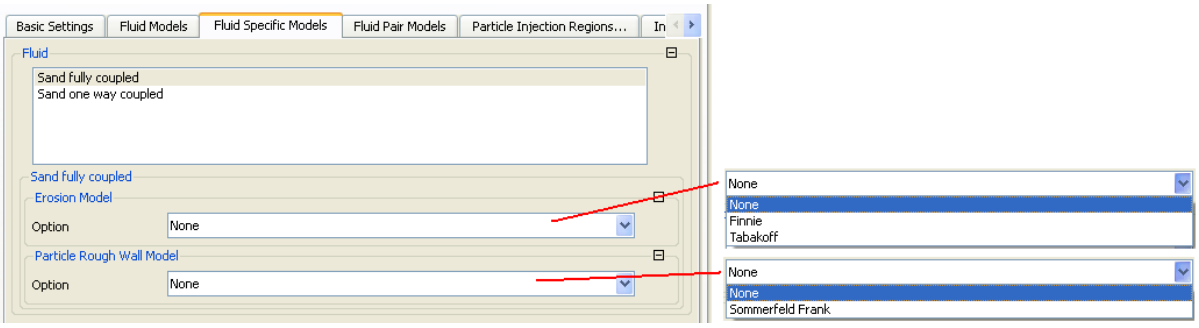
ANSYS CFX: DOMAIN → BASIC SETTINGS



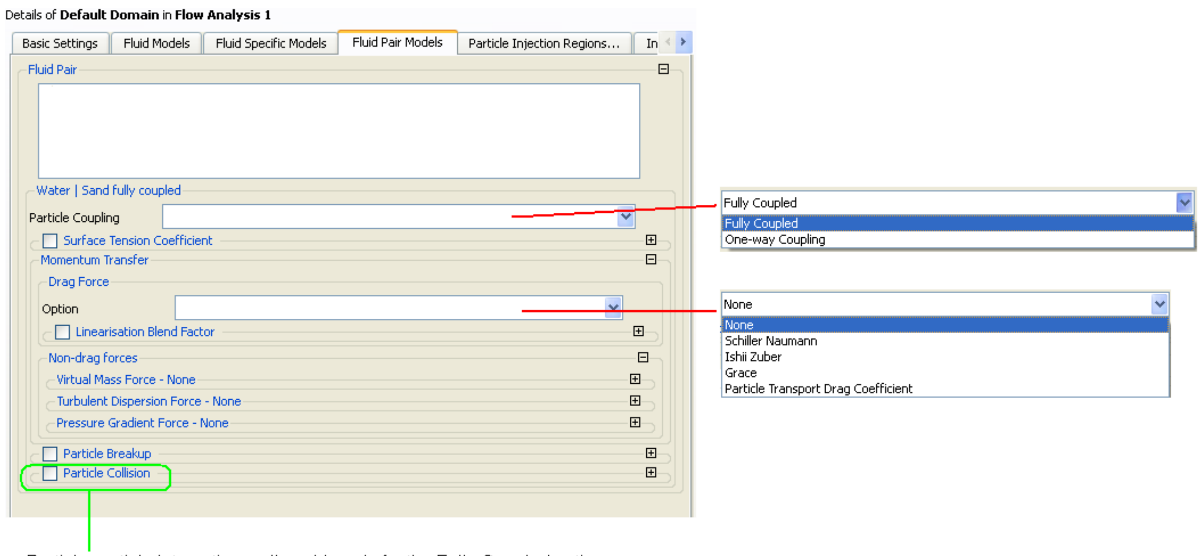
ANSYS CFX: DOMAIN → FLUID MODELS



ANSYS CFX: DOMAIN → FLUID SPECIFIC MODELS

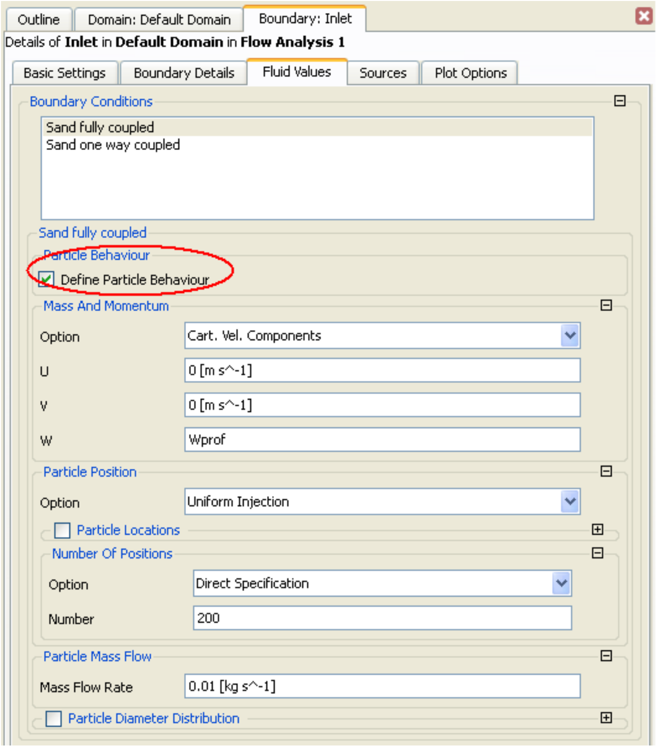


ANSYS CFX: DOMAIN → FLUID PAIR MODELS

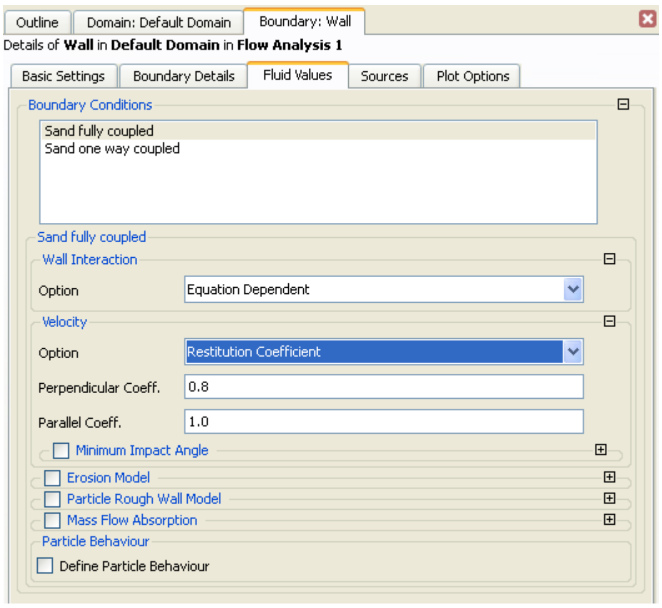


Particle-particle Interactions: allowable only for the Fully Coupled option

Ansys CFX: B.C. → Particles' injection



Ansys CFX: B.C. → Wall



Available tutorials in Ansys CFX

Available tutorials

n.	Description	Type
9	Free surface	Eulerian-Eulerian, Homogeneous
11	Butterfly valve	Eulerian-Lagrangian
		Particle Tracking
18	Airlift reactor	Eulerian-Eulerian, Inhomogeneous
		Bubble dispersion in water