

Lecture 14 - Multiphase Flows

Applied Computational Fluid Dynamics

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Definitions

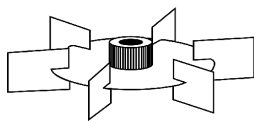
- Multiphase flow is simultaneous flow of:
 - Materials with different states or phases (i.e. gas, liquid or solid).
 - Materials with different chemical properties but in the same state or phase (i.e. liquid-liquid systems such as oil droplets in water).
- The primary and secondary phases:
 - One of the phases is continuous (primary) while the other(s) (secondary) are dispersed within the continuous phase.
 - A diameter has to be assigned for each secondary phase to calculate its interaction (drag) with the primary phase.
 - A secondary phase with a particle size distribution is modeled by assigning a separate phase for each particle diameter.

Definitions (2)

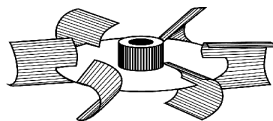
- Dilute versus dense phase:
 - Refers to the volume fraction of secondary phase(s).
 - Volume fraction of a phase = $\frac{\text{Volume of the phase in a cell/domain}}{\text{Volume of the cell/domain}}$
- Laminar versus turbulent:
 - Each phase can be laminar or turbulent.
 - Fluid flow (primary phase) may be turbulent with respect to the secondary phase but may be laminar with respect to the vessel.

Why model multiphase flow?

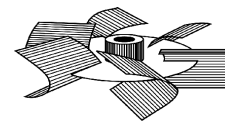
- Multiphase flow is important in many industrial processes:
 - Riser reactors.
 - Bubble column reactors.
 - Fluidized bed reactors.
 - Scrubbers, dryers, etc.
- Typical objectives of a modeling analysis:
 - Maximize the contact between the different phases, typically different chemical compounds.
 - Flow dynamics.



Rushton



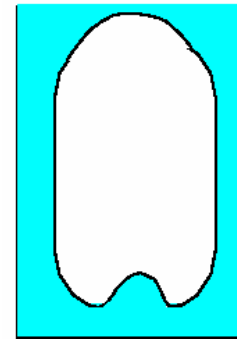
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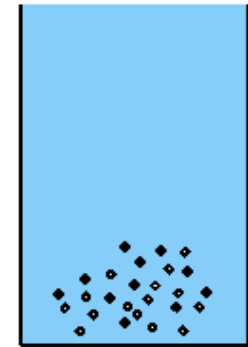
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Multiphase flow regimes

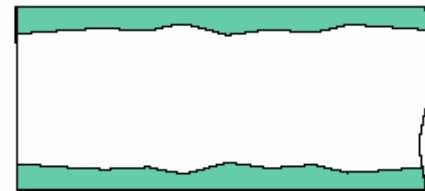
- Bubbly flow: discrete gaseous bubbles in a continuous liquid.
- Droplet flow: discrete fluid droplets in a continuous gas.
- Particle-laden flow: discrete solid particles in a continuous fluid.
- Slug flow: large bubbles in a continuous liquid.
- Annular flow: continuous liquid along walls, gas in core.
- Stratified and free-surface flow: immiscible fluids separated by a clearly-defined interface.



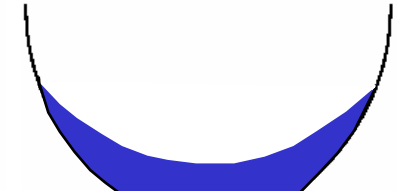
slug flow



bubbly flow
droplet flow
particle-laden flow

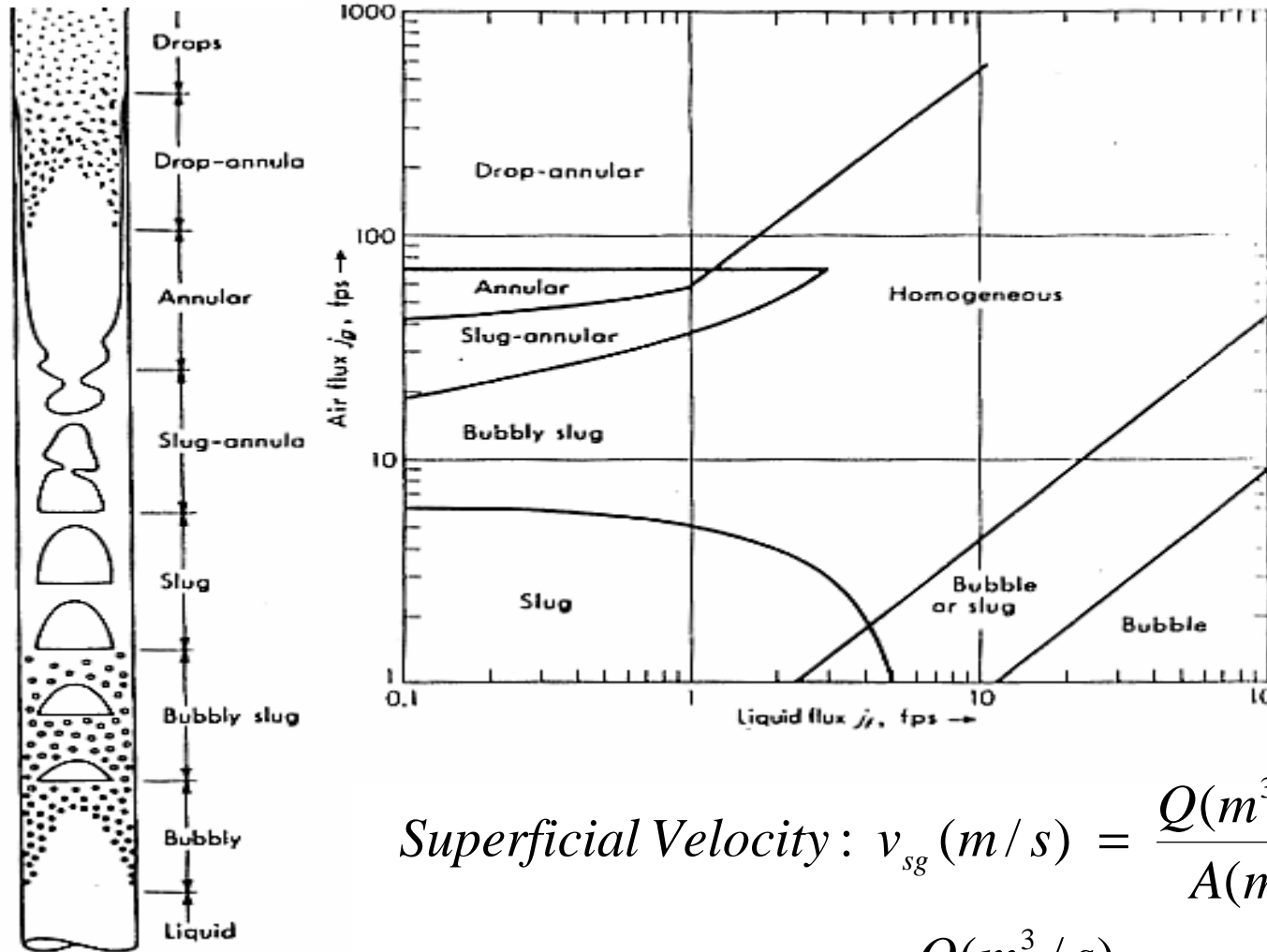


annular flow



free-surface flow

Flow regimes: vertical gas-liquid flow



Evaporator

$$\text{Superficial Velocity: } v_{sg} \text{ (m/s)} = \frac{Q \text{ (m}^3 \text{/s)}}{A \text{ (m}^2 \text{)}}$$

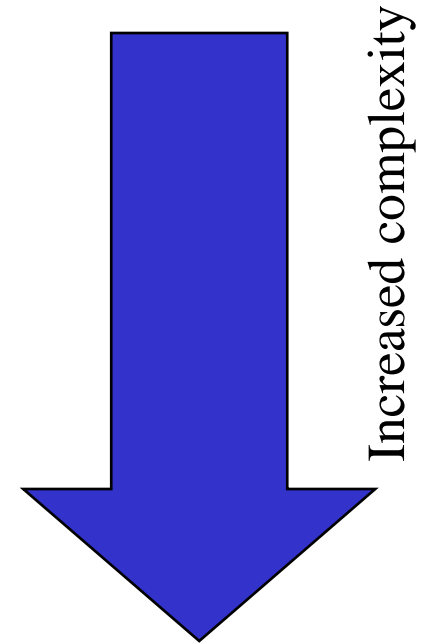
$$Q(\text{VVM}) = 60 \frac{Q \text{ (m}^3 \text{/s)}}{V \text{ (m}^3 \text{)}}$$

Multiphase flow regimes

- User must know a priori the characteristics of the flow.
- Flow regime, e.g. bubbly flow, slug flow, annular flow, etc.
- Only model one flow regime at a time.
- Predicting the transition from one regime to another possible only if the flow regimes can be predicted by the same model. This is not always the case.
- Laminar or turbulent.
- Dilute or dense.
- Secondary phase diameter for drag considerations.

Modeling approach

- Empirical correlations.
- Lagrangian.
 - Track individual point particles.
 - Particles do not interact.
- Algebraic slip model.
 - Dispersed phase in a continuous phase.
 - Solve one momentum equation for the mixture.
- Two-fluids theory (multi-fluids).
 - Eulerian models.
 - Solve as many momentum equations as there are phases.
- Discrete element method.
 - Solve the trajectories of individual objects and their collisions, inside a continuous phase.
- Fully resolved and coupled.

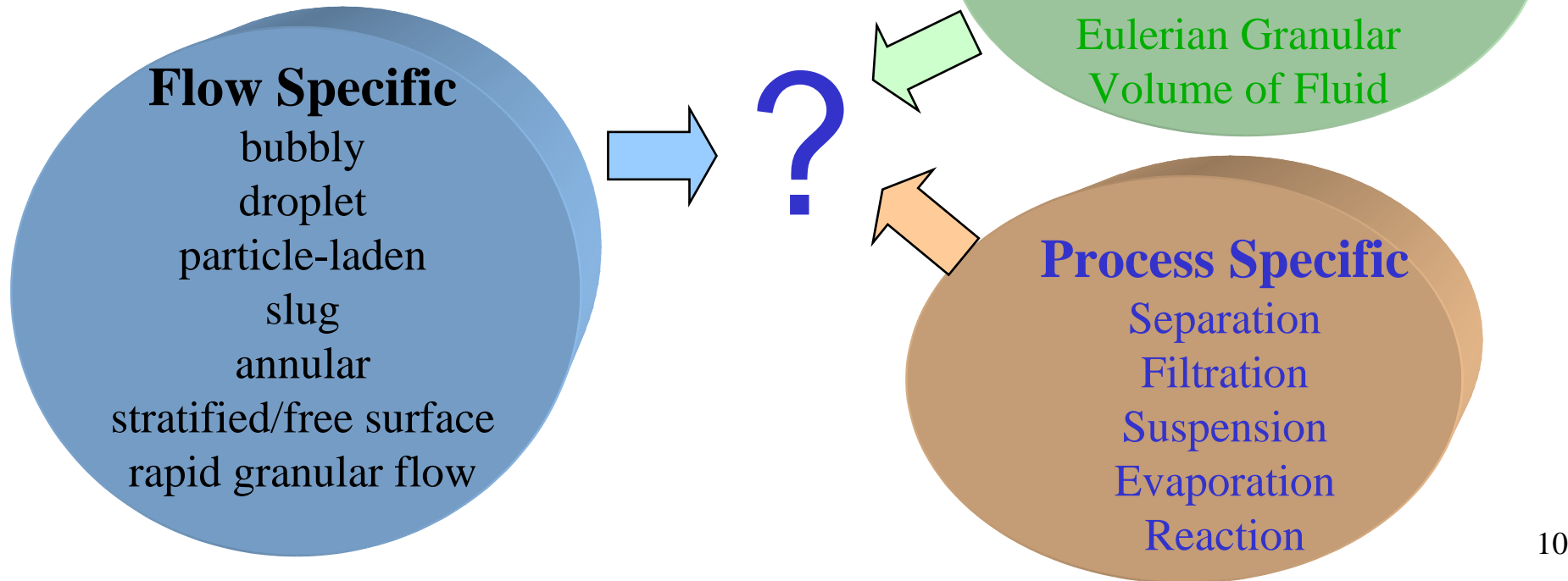


Coupling between phases

- One-way coupling:
 - Fluid phase influences particulate phase via aerodynamic drag and turbulence transfer.
 - No influence of particulate phase on the gas phase.
- Two-way coupling:
 - Fluid phase influences particulate phase via aerodynamic drag and turbulence transfer.
 - Particulate phase reduces mean momentum and turbulent kinetic energy in fluid phase.
- Four-way coupling:
 - Includes all two-way coupling.
 - Particle-particle collisions create particle pressure and viscous stresses.

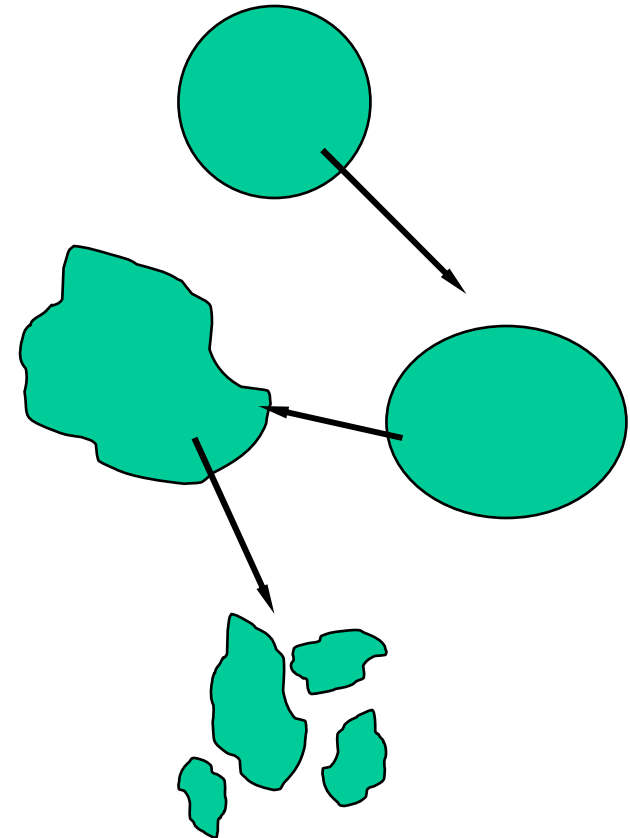
Modeling multiphase flows

- What is the goal of the simulation?
- Which effects are important?
- Controlled by which hydrodynamic effects?
- Controlled by which other transport phenomena effects?
- All these factors influence which model to choose for the analysis.



Physical effects in dispersed systems

- Hydrodynamics:
 - Change in shape.
 - Diameter.
 - Particle-wall collision.
 - Particle-particle collision.
 - Coalescence.
 - Dispersion and breakup.
 - Turbulence.
 - Inversion.
- Other transport phenomena:
 - Heat transfer.
 - Mass transfer.
 - Change in composition.
 - Heterogeneous reactions.



Hydrodynamics: particle relaxation time

- When does the particle follow the flow?
- Time when particle reaches about 60% of the initial difference velocity.

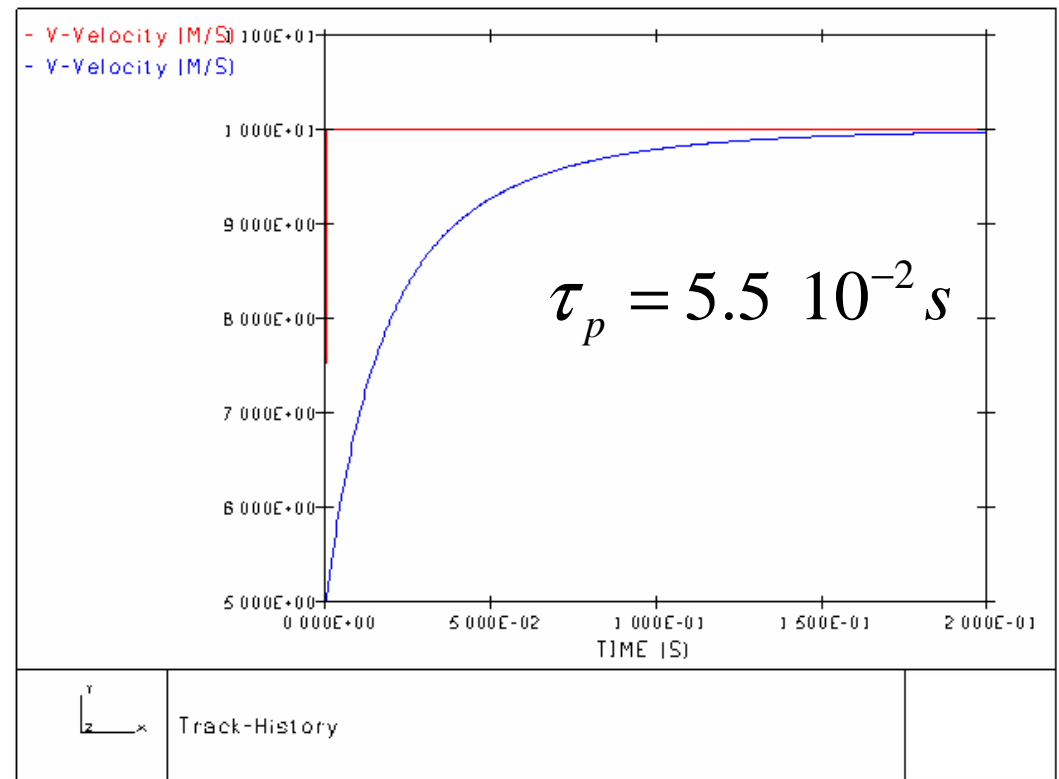
$$\tau_p = \frac{d_p^2 \rho_p}{18 \mu_g f_D}$$

$$d_p = 0.1 \text{ mm}$$

$$\rho_p = 1000 \text{ kg / m}^3$$

$$\mu_g = 1 \cdot 10^{-5} \text{ Pa s}$$

$$f_D = \text{Re}_p C_D / 24$$



Hydrodynamics: particle relaxation time

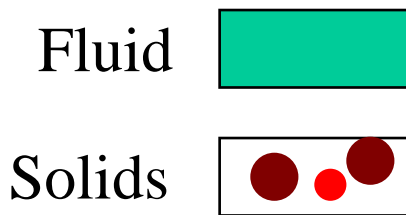
Typical relaxation times in process applications

	d_p	ρ_p	μ_g	τ_p
Coal combustion	1-500 μ	600-2000	2E-5 Pa s	1.7 E-6 – 1.4 s
Bubble columns	1-5 mm	1	1E-3 Pa s	5.5E-5 – 1.4E-3 s
Sand/air	0.1-5 mm	2000	2E-5 Pa s	5.5E-2 – 140 s
Sand/water	0.1-5 mm	2000	1E-3 Pa s	1E-3 – 2.7 s

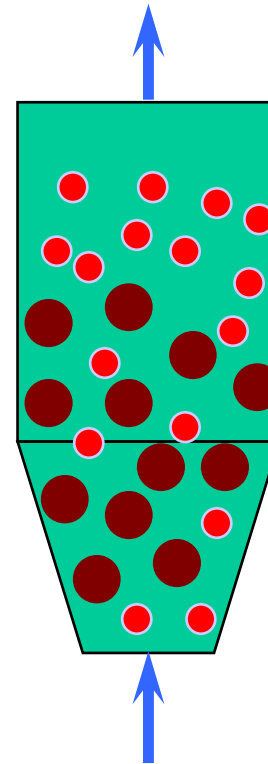
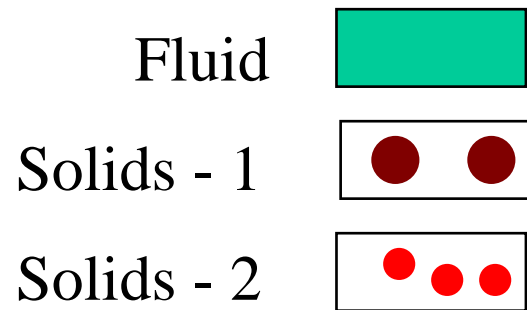
$$\tau_p = \frac{d_p^2 \rho_p}{18 \mu_g}$$

Multiphase formulation

- Two phases



- Three phases



Model overview

- Eulerian/Lagrangian dispersed phase model (DPM).
 - All particle relaxation times.
 - Particle-wall interaction always taken into account, particle-particle usually not.
- Algebraic Slip Mixture Model (ASM).
 - Particle relaxation times $< 0.001 - 0.01$ s.
 - Neither particle-wall interaction nor particle-particle are taken into account.
- Eulerian-Eulerian model (EEM).
 - All particle relaxation times.
 - Particle-wall interaction taken into account, particle-particle usually not.
- Eulerian-granular model (EGM).
 - All particle relaxation times.
 - Both particle-wall and particle-particle interaction are taken into account.

Algebraic slip model (ASM)

- Solves one set of momentum equations for the mass averaged velocity and tracks volume fraction of each fluid throughout domain.
- Assumes an empirically derived relation for the relative velocity of the phases.
- For turbulent flows, single set of turbulence transport equations solved.
- This approach works well for flow fields where both phases generally flow in the same direction.

ASM equations

- Solves one equation for continuity of the mixture:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = 0$$

- Solves for the transport of volume fraction of one phase:

$$\frac{\partial \alpha_2}{\partial t} + \frac{\partial u_{m,i} \alpha_2}{\partial x_i} = 0$$

- Solves one equation for the momentum of the mixture:

$$\frac{\partial}{\partial t} (\rho u_{m,j}) + \frac{\partial}{\partial x_i} \rho_m u_{m,i} u_{m,j} = - \frac{\partial P}{\partial x_j} +$$
$$\frac{\partial}{\partial x_i} \mu_{eff} \left(\frac{\partial u_{m,i}}{\partial x_j} + \frac{\partial u_{m,j}}{\partial x_i} \right) + \rho_m g_j + F_j + \frac{\partial}{\partial x_i} \sum_{k=1}^n \alpha_k \rho_k u_{k,i}^r u_{k,j}^r$$

ASM equations (2)

- Average density: $\rho_m = \alpha_1 \rho_1 + \alpha_2 \rho_2$
- Mass weighted average velocity: $\vec{u}_m = \frac{\rho_1 \alpha_1 \vec{u}_1 + \rho_2 \alpha_2 \vec{u}_2}{\rho_1 \alpha_1 + \rho_2 \alpha_2}$
- Velocity and density of each phase: $\vec{u}_1, \vec{u}_2, \rho_1, \rho_2$
- Drift velocity: $\vec{u}_1^r = \vec{u}_1 - \vec{u}_m$
- Effective viscosity: $\mu_{eff} = \mu_1 \alpha_1 + \mu_2 \alpha_2$

Slip velocity and drag

- Uses an empirical correlation to calculate the slip velocity between phases.

$$\Delta u = \vec{u}_{rel} = \vec{a} \tau_p$$

$$\vec{a} = (\vec{g} - (\vec{u}_m \cdot \nabla \vec{u}_m + \frac{\partial \vec{u}_m}{\partial t}))$$

$$\tau_p = \frac{(\rho_m - \rho_p) d_p^2}{18 \mu_f f_{drag}}$$

- f_{drag} is the drag function.

$$f_{drag} = \begin{cases} 1 + 0.15 \text{Re}^{0.687} & \text{if } \text{Re} \leq 1000 \\ 0.0175 \text{Re} & \text{if } \text{Re} > 1000 \end{cases}$$

Restrictions

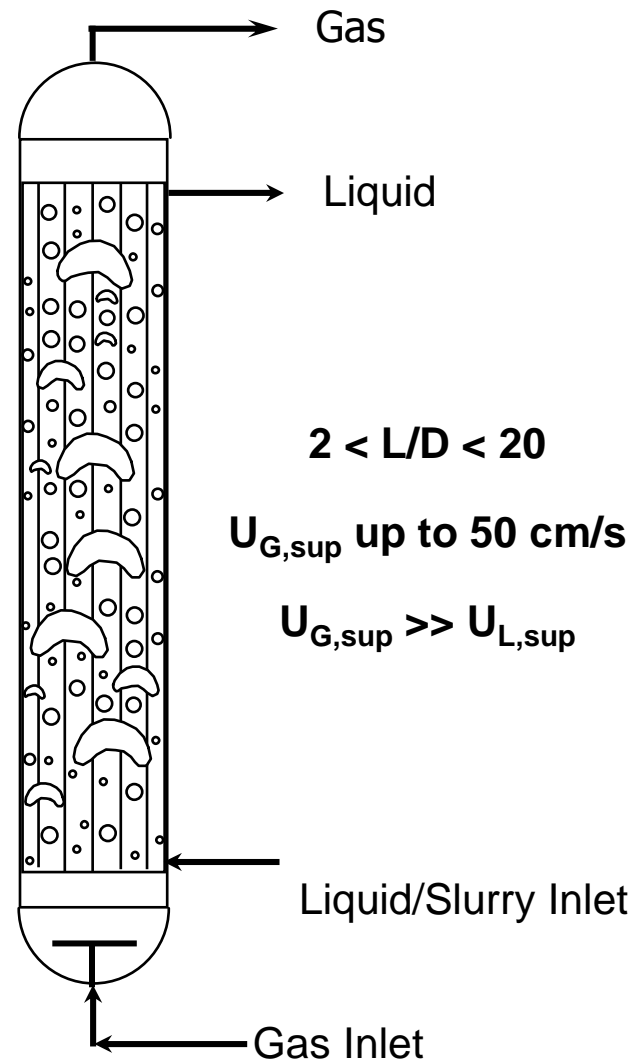
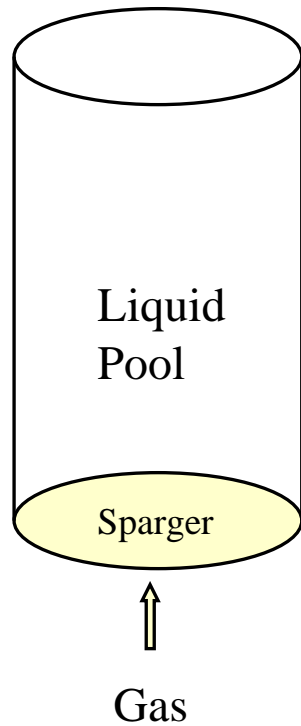
- Applicable to low particle relaxation times

$$\tau_p f_{drag} = \frac{(\rho_m - \rho_p)d_p^2}{18\mu_f} < 0.001 - 0.01s.$$

- One continuous phase and one dispersed phase.
- No interaction inside dispersed phase.
- One velocity field can be used to describe both phases.
 - No countercurrent flow.
 - No sedimentation.

Example: bubble column design

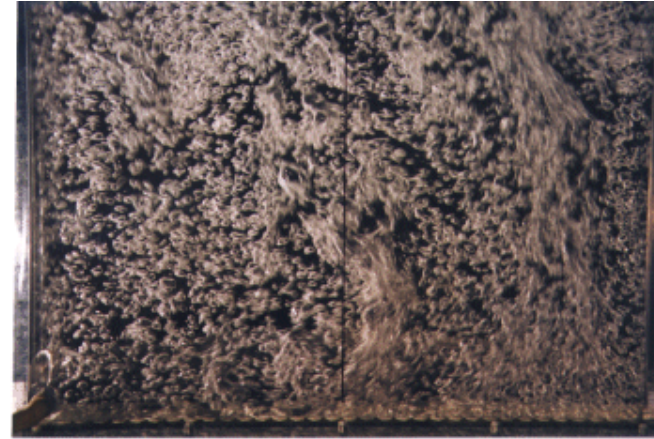
A bubble column is a liquid pool sparged by a process stream.



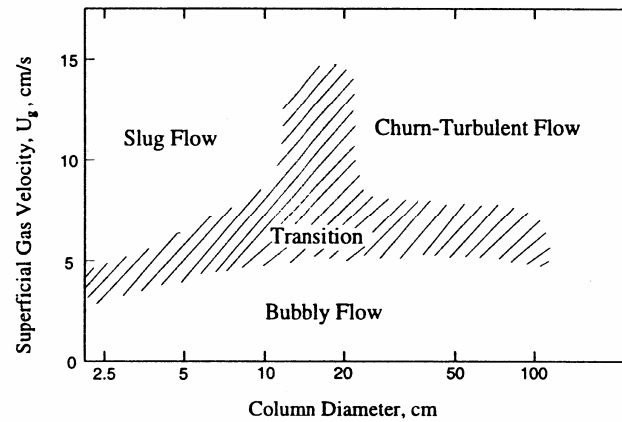
Bubble columns: flow regimes



Bubbly Flow



Churn-Turbulent Flow ("Heterogeneous")



Flow Regime Map (Deckwer, 1980)

Bubble column design issues

- Design parameters:
 - Gas holdup. Directly related to rise velocity. Correlations of the form $\alpha \sim u_{sg}^a \rho_l^b \sigma^c \mu_l^d$ are commonly used.
 - Mass transfer coefficient $k_1 a$. Correlations of the form $k_1 a \sim u_{sg}^a \rho_l^b \sigma^c \mu_l^d \mu_g^e D^f \Delta \rho^g$ are commonly used.
 - Axial dispersion occurs in both the liquid and gas phase, and correlations for each are available.
 - Mixing time. Correlations are available for a limited number of systems.
 - Volume, flow rates and residence time.
 - Flow regime: homogeneous, heterogeneous, slug flow.

Bubble column design issues - cont'd

- Accurate knowledge of the physical properties is important, especially the effects of coalescence and mass transfer affecting chemicals.
- Although good correlations are available for commonly studied air-water systems, these are limited to the ranges studied.
- Correlations may not be available for large scale systems or systems with vessel geometries other than cylinders without internals.
- Furthermore, experimental correlations may not accurately reflect changes in performance when flow regime transitions occur.

Bubble size

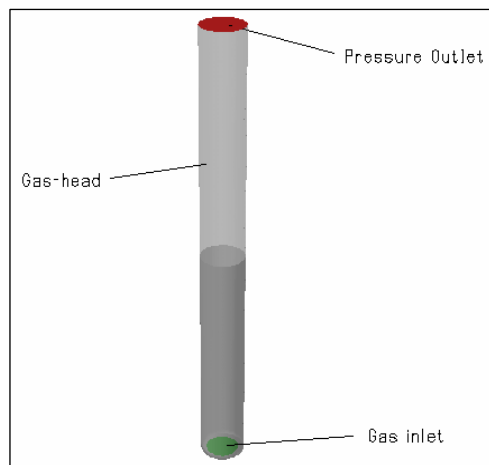
- At present, bubble column reactors are modeled using a single effective bubble size.
- Coalescence and breakup models are not yet mature.
- Statistical approach. Solve equation for number density.
- Population balance approach.
 - Application of population balance with two-fluid models with initial focus on gas-liquid.
 - The gas phase is composed of n bubble bins and share the same velocity as the second phase.
 - The death and birth of each bubble bin is solved from the above models.

Model setup

- The flow in bubble column reactors is typically modeled as being transient.
- The time step used in the transient calculation needs to be small enough to capture the phenomena of interest and large enough to reduce CPU time. A typical time step would be of the order of $1E-3$ times the gas residence time.
- Typically use standard k- ϵ model for turbulence.
- Use PISO.
- First order differencing for all variables except volume fraction (second order) and in time.
- Typical underrelaxation factors 0.5 for pressure, 0.2 for momentum, 0.8 for turbulence, 0.1 for slip velocity (with ASM model), and 0.5 for volume fraction.
- Initialization of gas volume fraction is not recommended. Start with $\alpha=0$.
- Don't forget to turn on gravity:-)
- Turn on implicit body force treatment (in operating conditions panel).
- Set reference density, but exact value of reference density is not crucial. Generally set to that of the lighter phase.

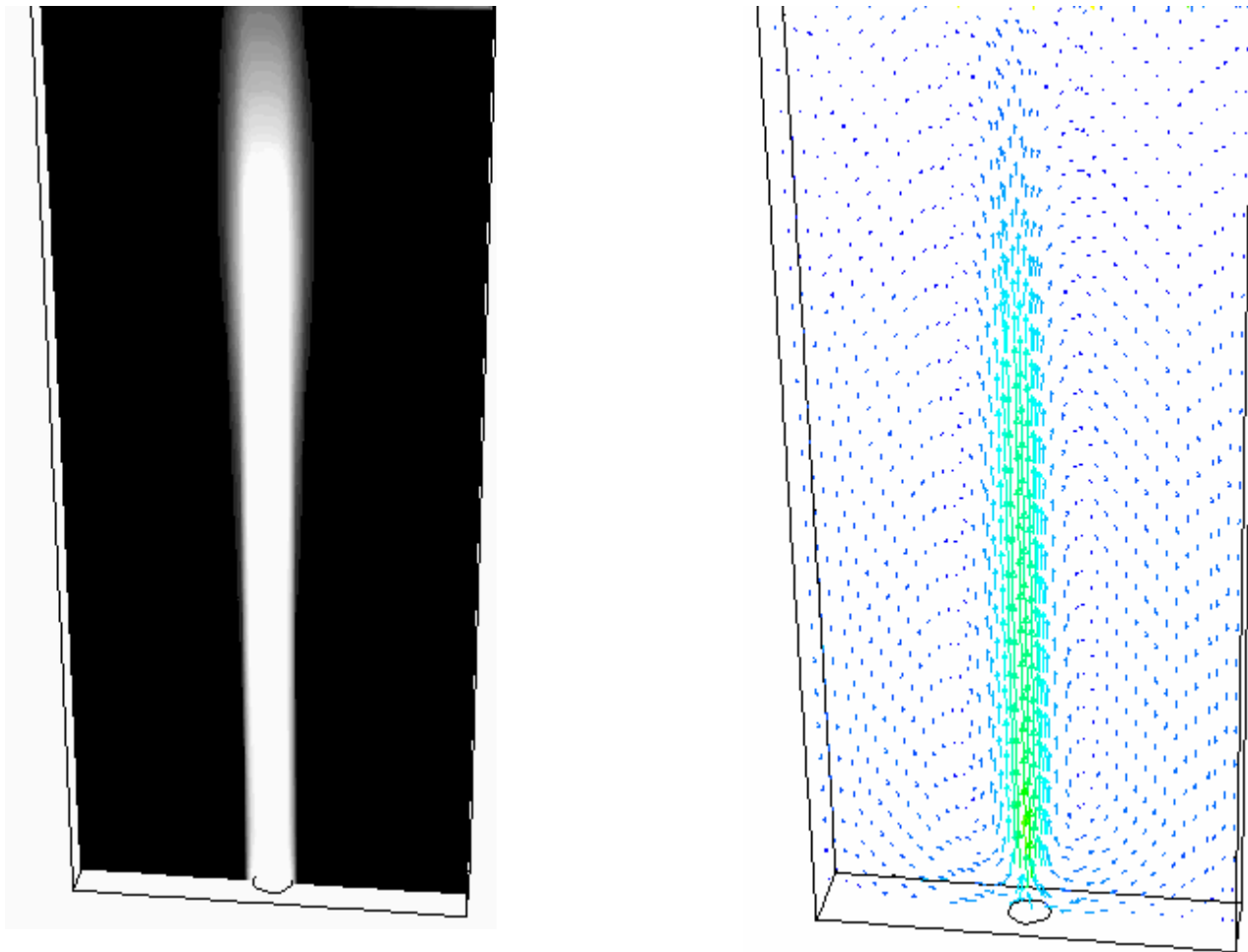
Bubble column example - ASM

- 3D modeling of dynamic behavior of an air-water churn turbulent bubble-column using the ASM model.
- This model solves only one momentum equation for the gas-liquid mixture.
- Constant bubble size is used.



Iso-contours of gas volume fraction

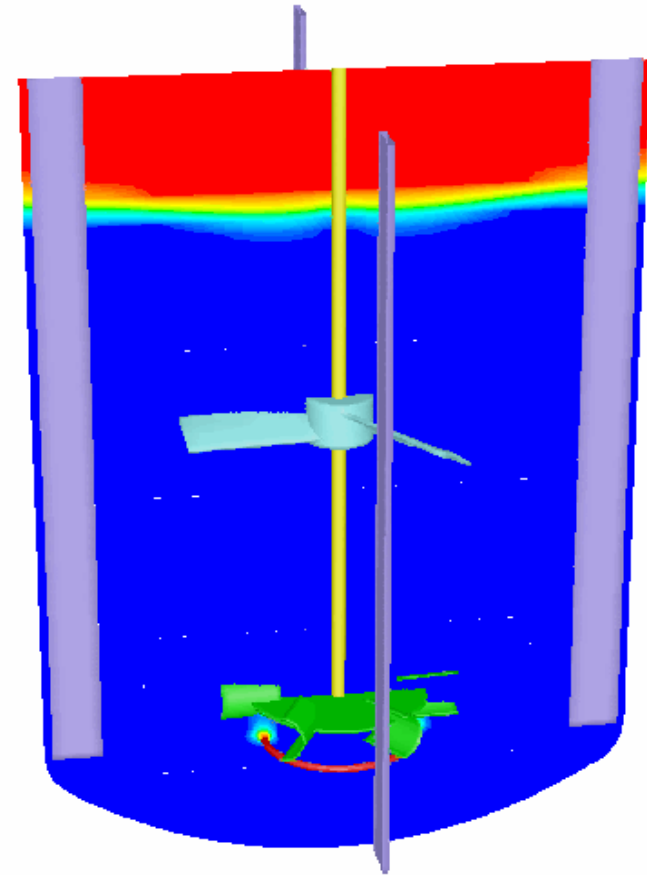
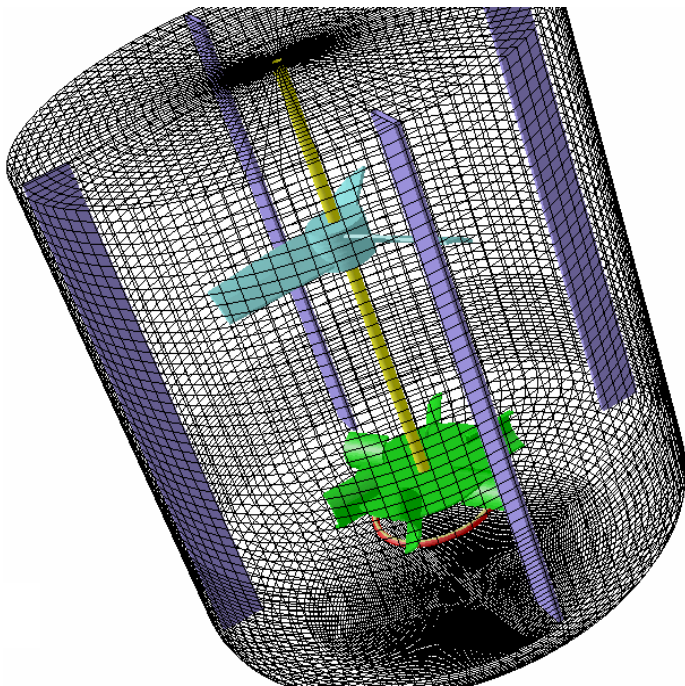
Bubble column example - ASM



Unstable flow in a 3-D bubble column with rectangular cross section.

Example - gas-liquid mixing vessel

- Combinations of multiple impeller types used.
- Bottom radial flow turbine disperses the gas.
- Top hydrofoil impeller provides good blending performance in tall vessels.



Eulerian Gas-Liquid Simulation
Animation

Eulerian-granular/fluid model features

- Solves momentum equations for each phase and additional volume fraction equations.
- Appropriate for modeling fluidized beds, risers, pneumatic lines, hoppers, standpipes, and particle-laden flows in which phases mix or separate.
- Granular volume fractions from 0 to ~60%.
- Several choices for drag laws. Appropriate drag laws can be chosen for different processes.
- Several kinetic-theory based formulas for the granular stress in the viscous regime.
- Frictional viscosity based formulation for the plastic regime stresses.
- Added mass and lift force.

Eulerian-granular/fluid model features

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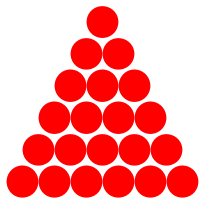
Granular flow regimes

Elastic Regime

Stagnant

Stress is strain
dependent

Elasticity

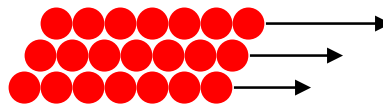


Plastic Regime

Slow flow

Strain rate
independent

Soil mechanics

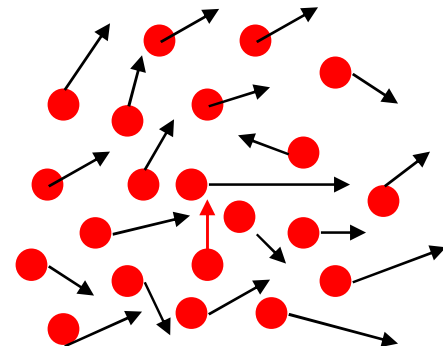


Viscous Regime

Rapid flow

Strain rate
dependent

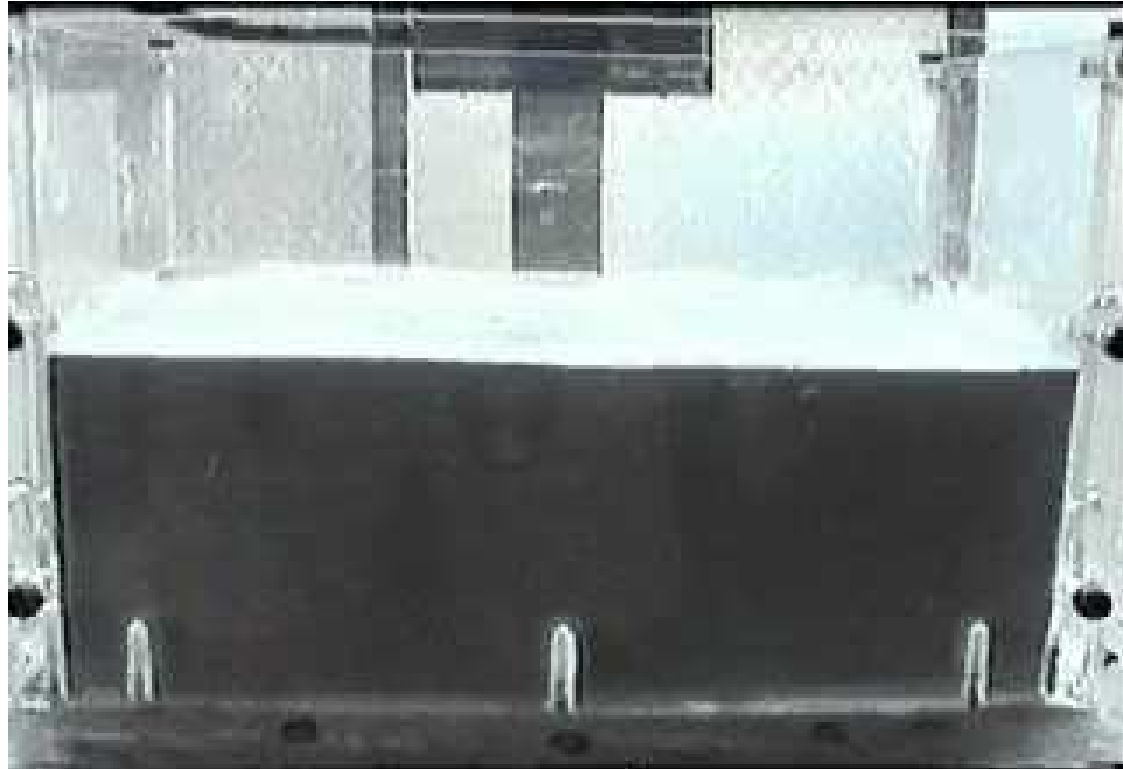
Kinetic theory



Fluidized-bed systems

- When a fluid flows upward through a bed of solids, beyond a certain fluid velocity the solids become suspended. The suspended solids:
 - has many of the properties of a fluid,
 - seeks its own level (“bed height”),
 - assumes the shape of the containing vessel.
- Bed height typically varies between 0.3m and 15m.
- Particle sizes vary between 1 μm and 6 cm. Very small particles can agglomerate. Particle sizes between 10 μm and 150 μm typically result in the best fluidization and the least formation of large bubbles. Addition of finer size particles to a bed with coarse particles usually improves fluidization.
- Superficial gas velocities (based on cross sectional area of empty bed) typically range from 0.15 m/s to 6 m/s.

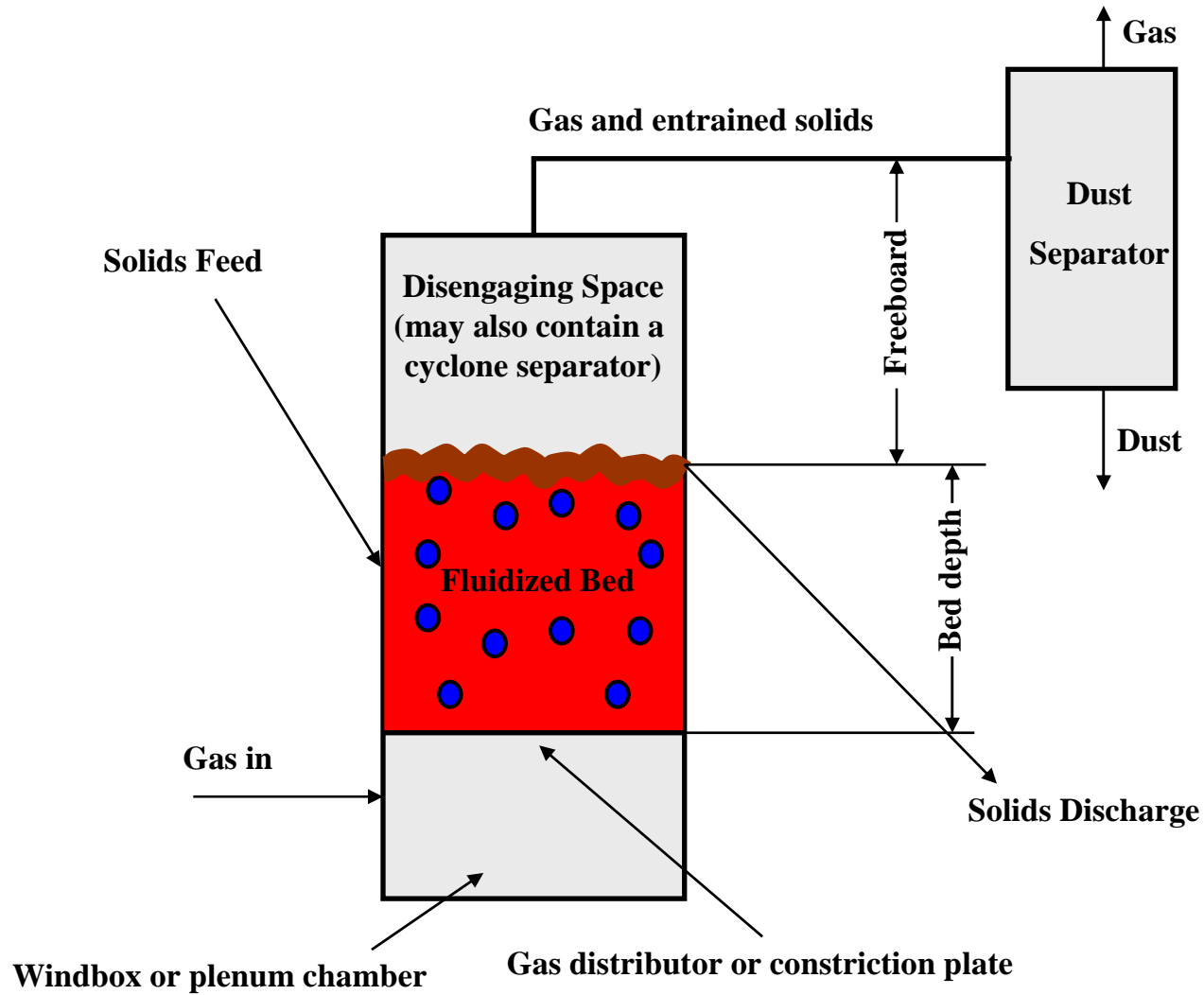
Fluidized bed example



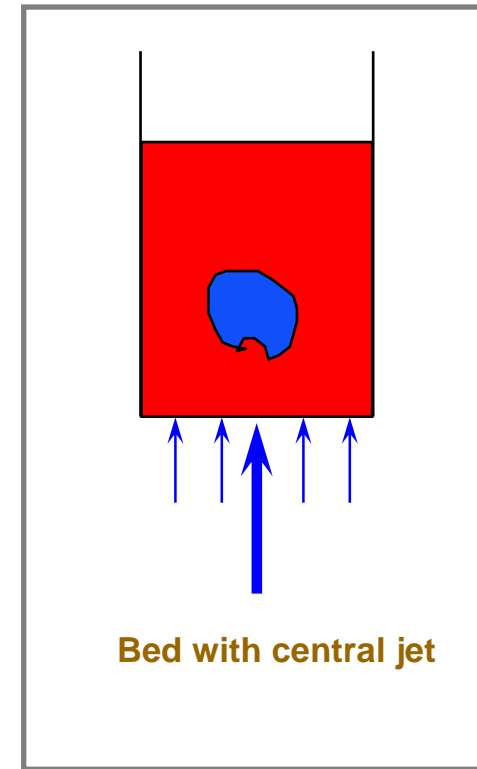
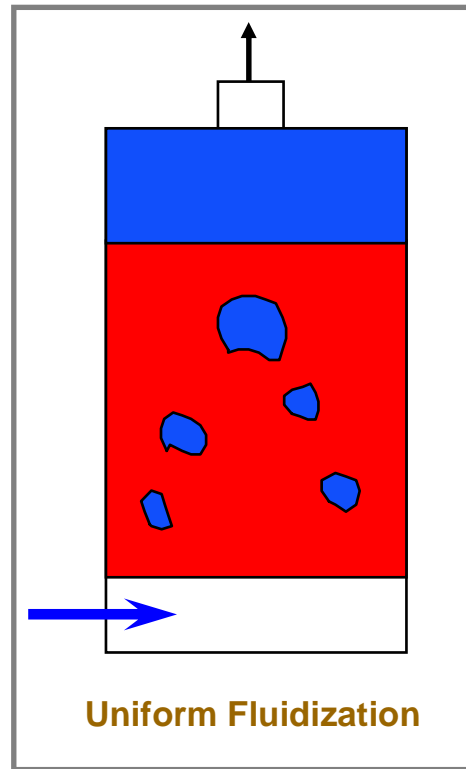
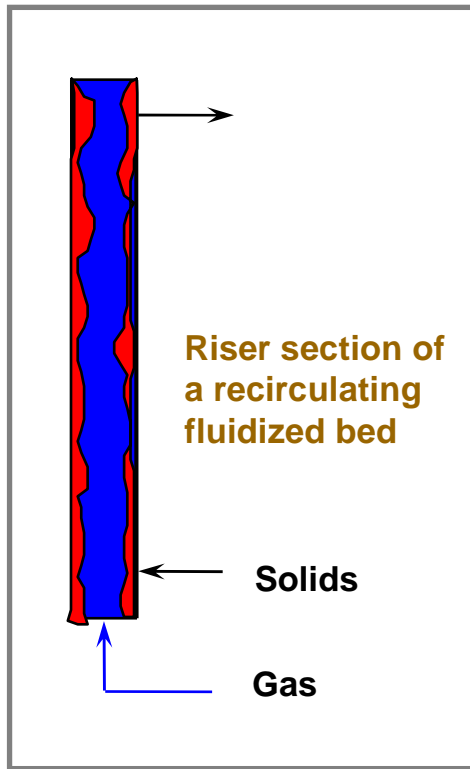
Fluidized bed uses

- Fluidized beds are generally used for gas-solid contacting. Typical uses include:
 - Chemical reactions:
 - Catalytic reactions (e.g. hydrocarbon cracking).
 - Noncatalytic reactions (both homogeneous and heterogeneous).
 - Physical contacting:
 - Heat transfer: to and from fluidized bed; between gases and solids; temperature control; between points in bed.
 - Solids mixing.
 - Gas mixing.
 - Drying (solids or gases).
 - Size enlargement or reduction.
 - Classification (removal of fines from gas or fines from solids).
 - Adsorption-desorption.
 - Heat treatment.
 - Coating.

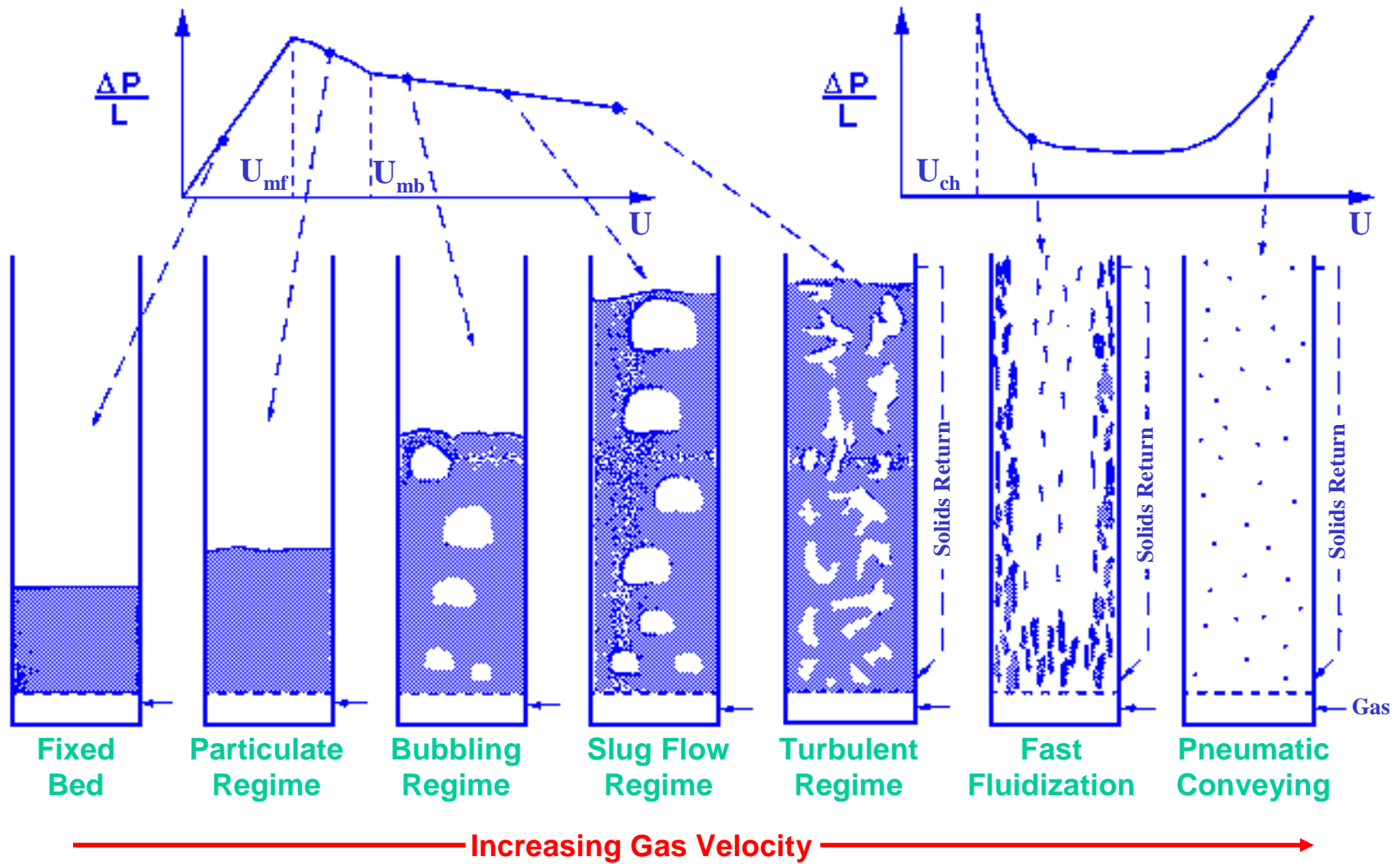
Typical fluidized bed systems - 1



Typical fluidized bed systems - 2



Fluidization regimes



Fluidized bed design parameters

- Main components are the fluidization vessel (bed portion, disengagement space, gas distributor), solids feeder, flow control, solids discharge, dust separator, instrumentation, gas supply.
- There is no single design methodology that works for all applications. The design methodologies to be used depend on the application.
- Typical design parameters are bed height (depends on gas contact time, solids retention time, L/D for staging, space required for internal components such as heat exchangers).
- Flow regimes: bubbling, turbulent, recirculating, slugs. Flow regime changes can affect scale-up.
- Heat transfer and flow around heat exchanger components.
- Temperature and pressure control.
- Location of instrumentation, probes, solids feed, and discharges.

Fluidized bed - input required for CFD

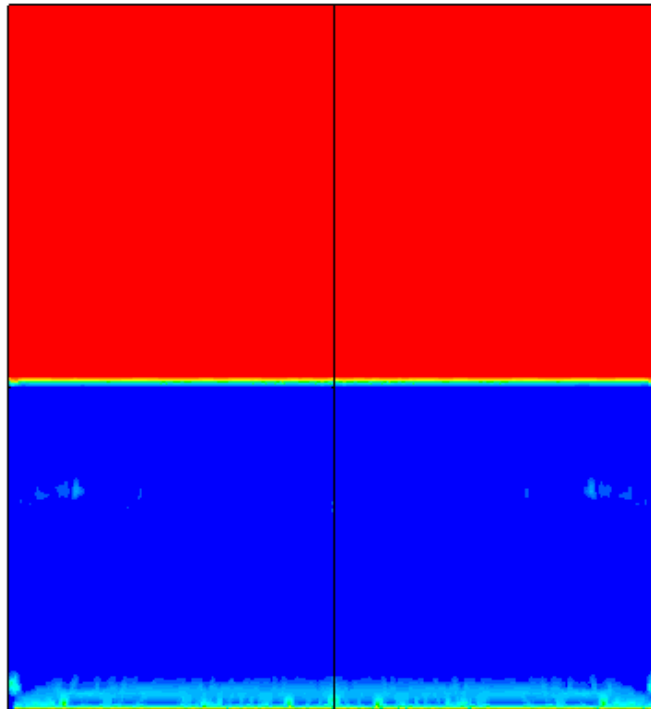
- CFD can not be used to predict the:
 - minimum fluidization velocity,
 - and the minimum bubbling velocity.
- These depend on the:
 - particle shape,
 - particle surface roughness,
 - particle cohesiveness, and the
 - particle size distribution.
- All of these effects are lumped into the drag term. Hence we need to fine tune the drag term to match the experimental data for minimum fluidization or minimum bubbling velocity.

Fluidized bed - when to use CFD

- If the drag term is tuned to match the minimum fluidization velocity, CFD then can be used to predict:
 - bed expansion
 - gas flow pattern
 - solid flow pattern
 - bubbling size, frequency and population
 - short circuiting
 - effects of internals
 - effects of inlet and outlets
 - hot spots
 - reaction and conversion rates
 - mixing of multiple particle size
 - residence times of solids and gases
 - backmixing and downflows (in risers)
 - solids distribution/segregation

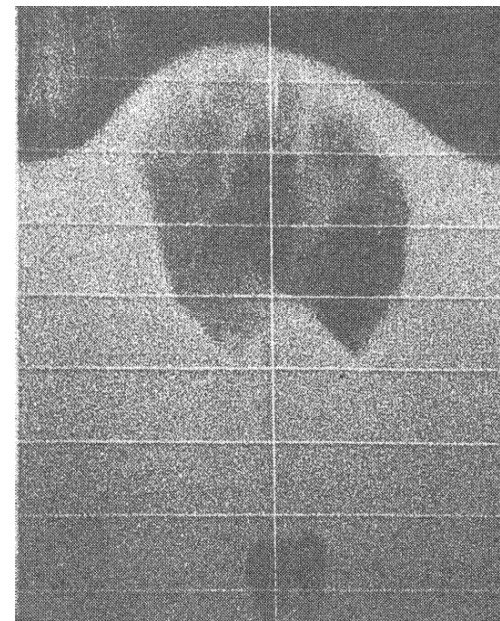
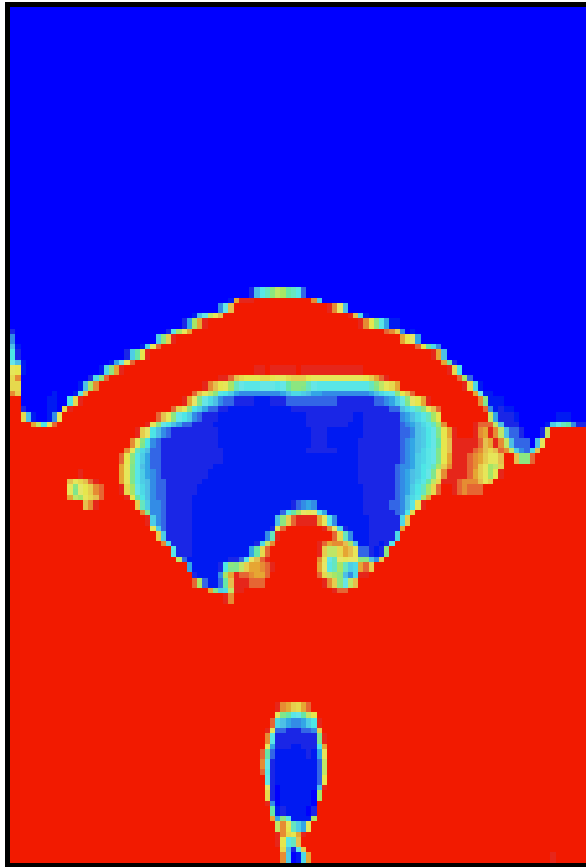
Fluidized bed animation

VOF of gas



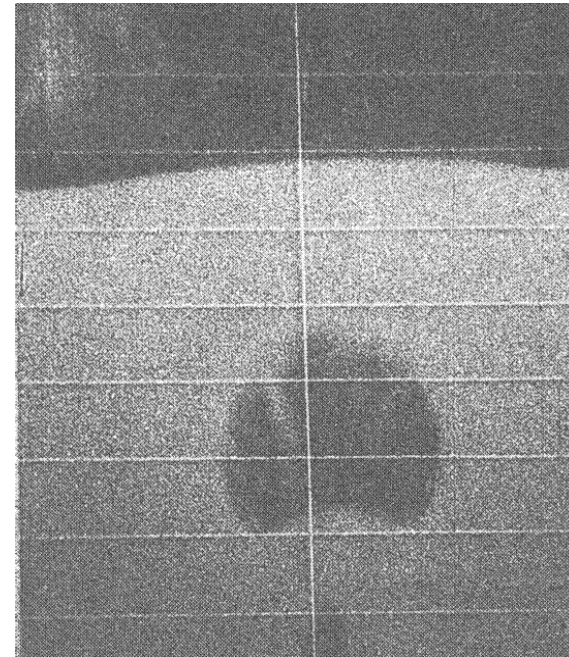
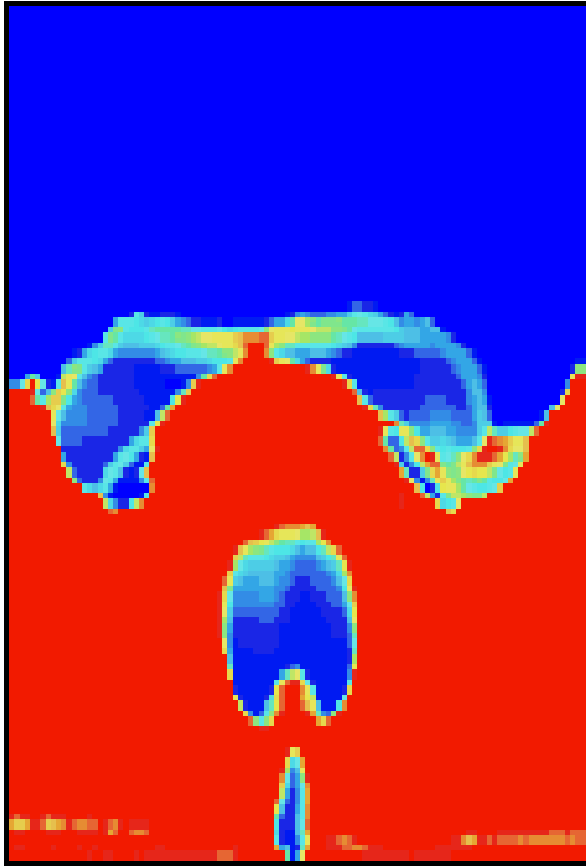
$V_s = 6 \text{ cm/s}$

Bubble size and shape - validation



Gidaspow (1994)

Bubble size and shape - validation



Gidaspow (1994)

Solution recommendations

- Use unsteady models for dense gas-solid flows (fluidized beds as well as dense pneumatic transport lines/risers). These flows typically have many complex features, and a steady state solution may not be numerically feasible unless a diffusive turbulence model (e.g. $k-\epsilon$) is used.
- Use small time steps (0.001 to 0.1s) to capture important flow features.
- Always tune the drag formula for the specific applications, to match the minimum fluidization velocity.
- Broadly speaking, the Gidaspow model is good for fluidized beds and Syamlal's model is good for less dense flows.
- Higher order discretization schemes give more realistic bubble shapes, as do finer grids.

Conclusion

- Today discussed the:
 - The algebraic slip model solves one momentum equation for the mixture.
 - Eulerian model solves one momentum equation per phase.
- In next lectures we will discuss particle tracking and free surface models.