Applications of Computational Fluid Dynamics in the Process Industries

Ahmad Haidari & Peter Spicka

Fluent Inc.

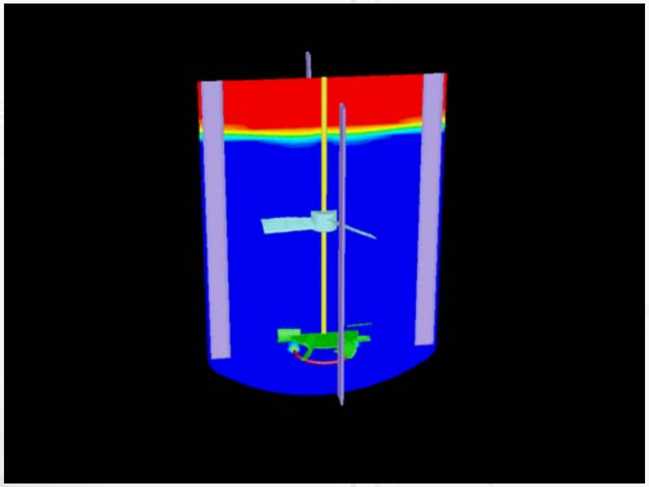
CREL meeting 2005

Outline

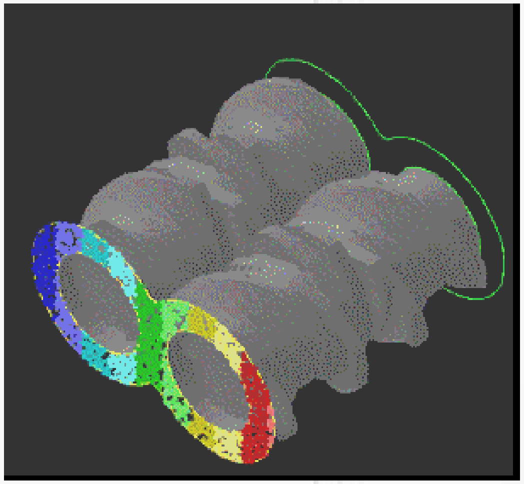
- Overview of CFD's growth in the process Industry
- Overview of modeling multiphase models in CFD
- Examples of Industrial use of CFD
  - Mixing
  - Particulate flows
  - Gas-liquid systems
- Solving population balance and CFD
- Summary

CFD is taking roots in the process industries

- CFD is used in many sections of the process industry helping to meet a diverse modeling need of clients wanting to do complex physics in complex geometries.



Gas-liquid mixing tank, FLUENT



Particle traces in an intermeshing gear pump POLYFLOW

CFD Applications in Chemical Industry

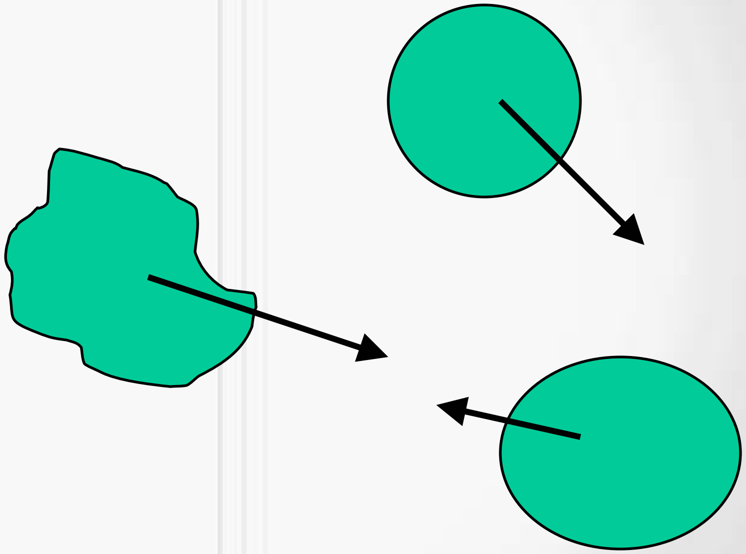
(Example-list)

- **Flow distribution devices** (Manifolds, Plates, Feed pipes, Injectors, Piping junctions)
- **Control and measurement** (Valves: positive displacement, gate, butterfly, ball)
- **Rotating machinery** (Pumps, Compressors, Fans, Discs, Seals, Turbines, Centrifuges, Mills)
- **Filtration**
- **Gravitational separators** (Cyclones, Hydrocyclone, knockout drums, Decanters, etc.)
- **Heat transfer and combustion equipments** (heat exchangers, Boilers, Combustors, Incineration, etc.)
- **Multiphase reactors** (Stirred tank, Bubble column, Tubular,Fixed bed, Fluidized beds, Slurry, Trickle bed)
- **Distillation** (Packed beds, Structure packing, Trays, Extraction column)
- **Dryers** (Fluidized bed, Ovens, Spray dryers, Rotary, Web dryers)
- **Polymer processing** (Extrusion, Coding, ..)
- **Particulate flows**
- **Safety, air Quality and clean room design**

Multiphase Flow Modeling with CFD

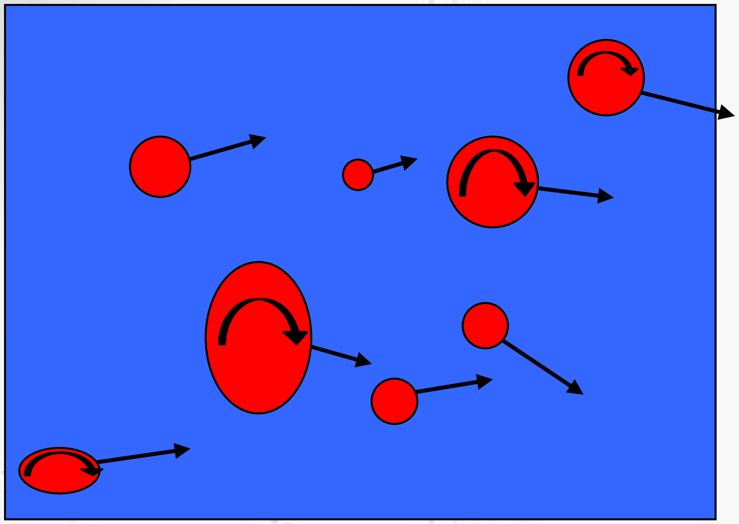
What are we interested in?

- Overall flow pattern
- Hydrodynamics
  - change in shape
  - diameter
  - coalescence
  - turbulence
- Heat and mass transfer
  - heat transfer
  - mass transfer & reaction rates
  - change in composition



CREL meeting 2005

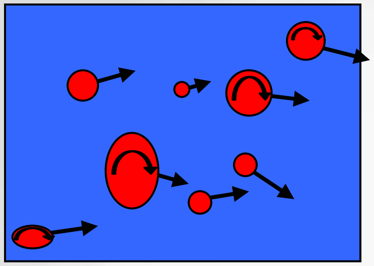
Multiphase Flow Models

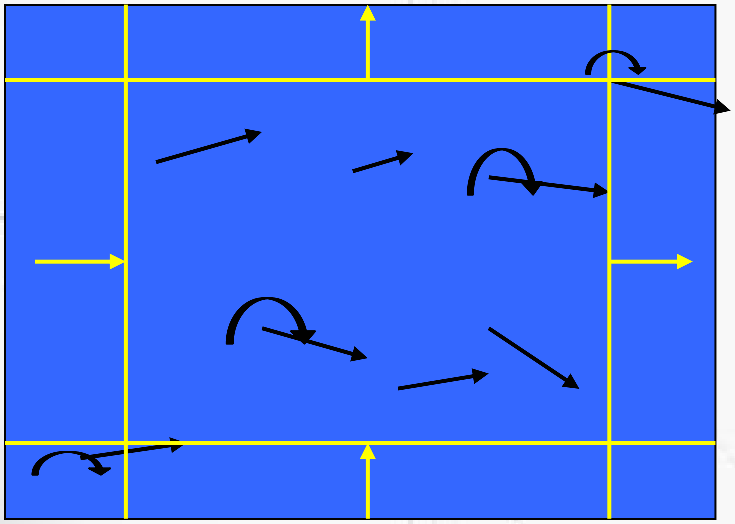


A suite of models was established in the past to consider:

- Pure hydrodynamics
- Voidage
- Size distributions
- Non-sphericity
- Rotation
- Collisions
- ...

Euler/Lagrange Model

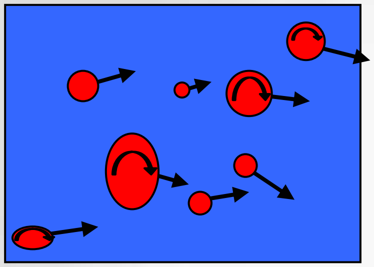


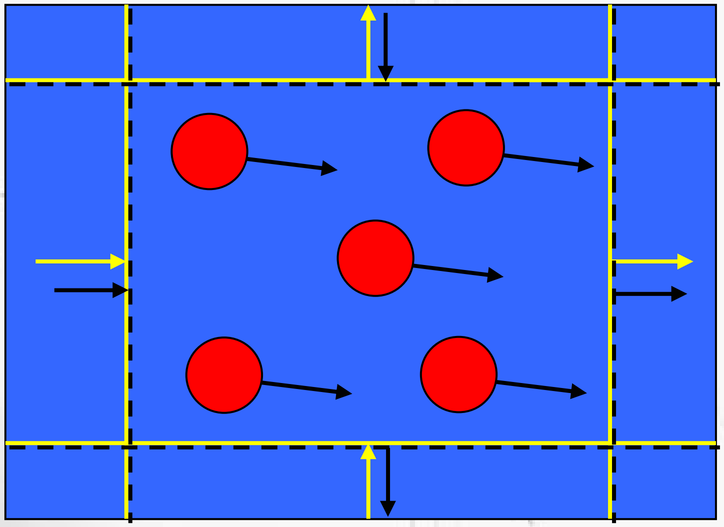


- CFD for fluid flow
- Detailed simulation of reference particles
- Particles act as mass points
- All effects need to be modelled

- Standard model in a lot of CFD-codes

Euler/Euler Model





- CFD for fluid flow
- CFD for dispersed flow

$$\frac{\partial \alpha_q}{\partial t} + \nabla \cdot (\alpha_q \vec{u}_q) = \frac{1}{\rho_q}\left(\sum_{p=1}^{n} \dot{m}_{pq} - \alpha_q \frac{\mathrm{d}\rho_q}{\mathrm{d}t}\right)$$

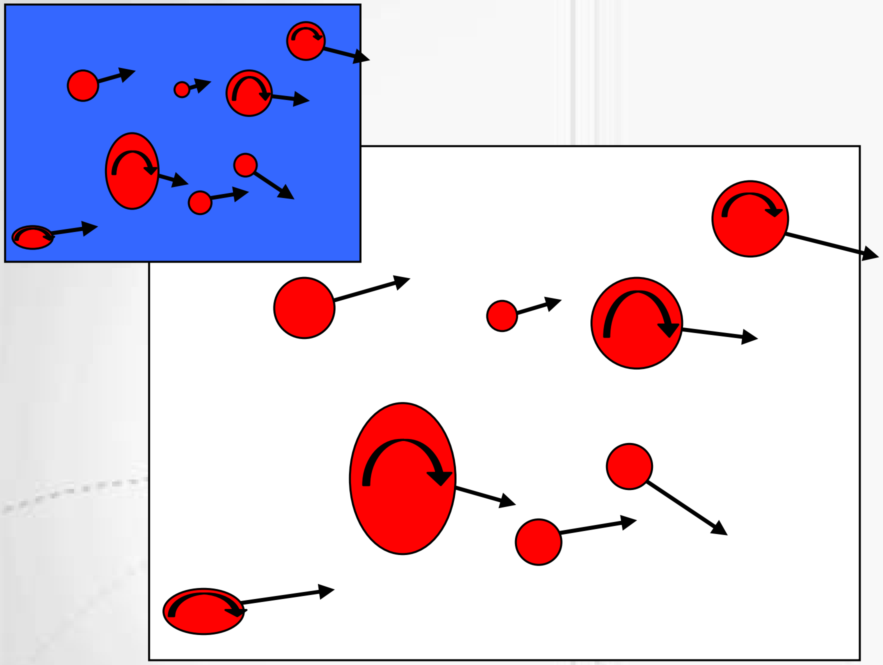
$$\frac{\partial}{\partial t}(\alpha_q \rho_q \vec{u}_q) + \nabla \cdot (\alpha_q \rho_q \vec{u}_q \vec{u}_q) = -\alpha_q \nabla p + \nabla \cdot \tau_q + \alpha_q \rho_q \vec{g} +$$

$$\alpha_q \rho_q \left(\vec{F}_q + \vec{F}_{lift,q} + \vec{F}_{vm,q}\right) + \sum_{p=1}^{n} \left(K_{pq}(\vec{u}_p - \vec{u}_q) + \dot{m}_{pq}\vec{u}_{pq}\right)$$

- Sub models available for
  - Heat/mass transfer
  - Cavitation
  - Kinetic theory of granular media
  - Population balances

FLUENT
The Right Answer in CFD

Discrete Models



- Detailed simulation of ALL particles
- Averaging on CFD-mesh
- Rotation

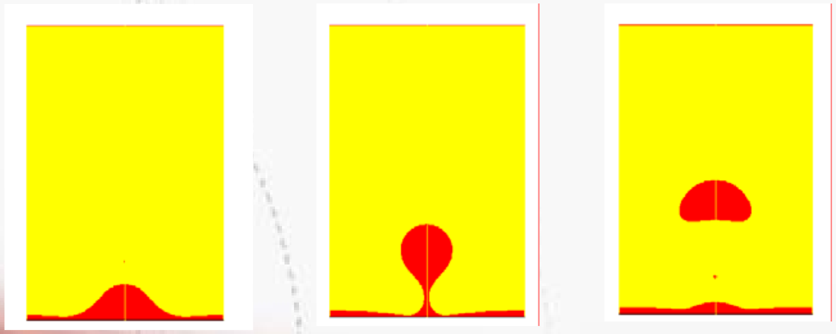
- Collisions with wall and other particles.

Examples:

- FLUENT‘s macroscopic particle model
- Discrete Element Method (DEM)

The Volume of Fluid Model (VOF)

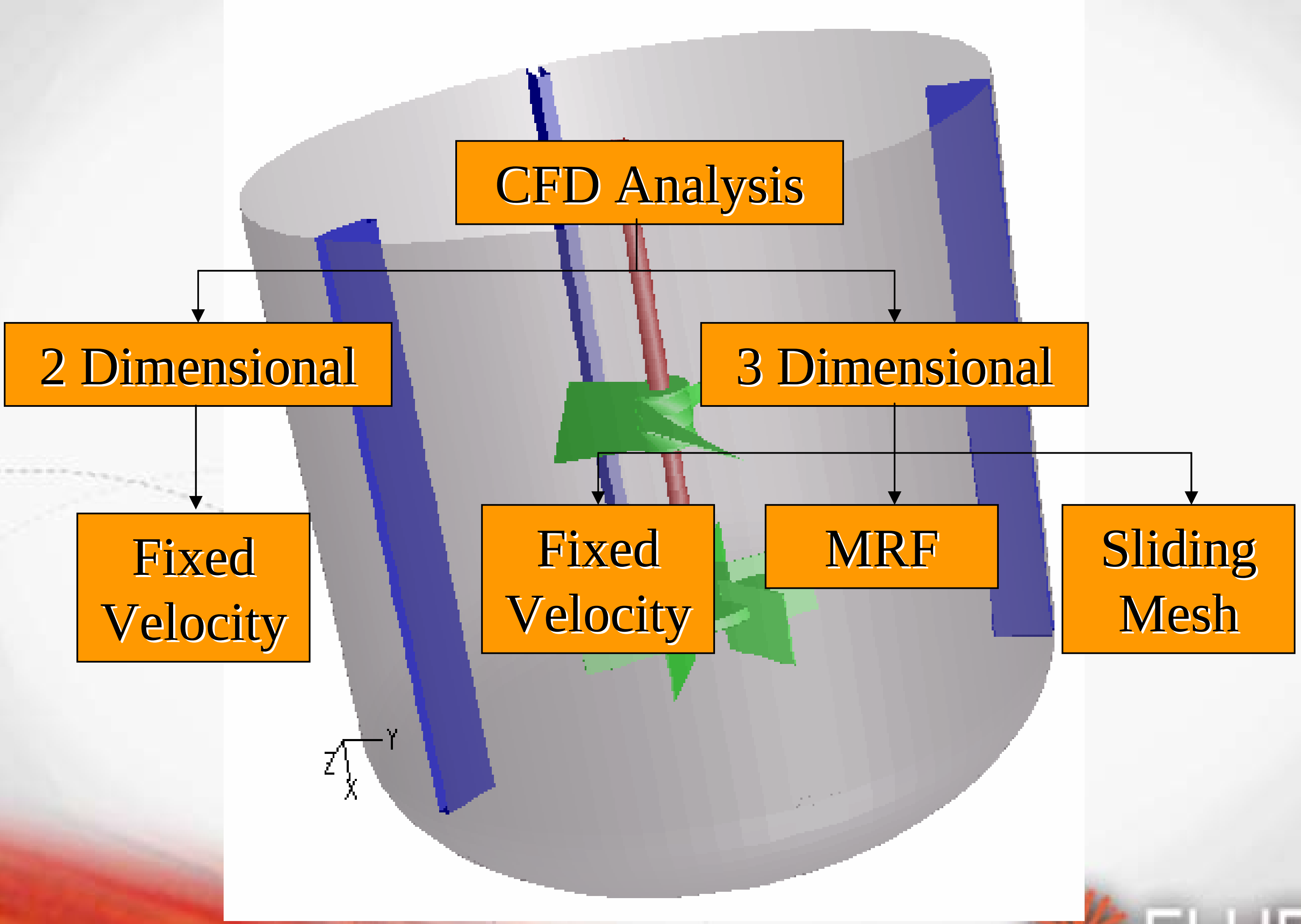
- The VOF model is designed to track the position of the interface between two or more immiscible fluids.
- A single momentum equation is solved and the resulting velocity field is shared by all phases.
  - Surface tension and wall adhesion effects can be taken into account.
  - Heterogeneous mass transfer (bubble formation, dissolution..)
- Solves transport equation for volume fraction of each secondary phase.



Film boiling example

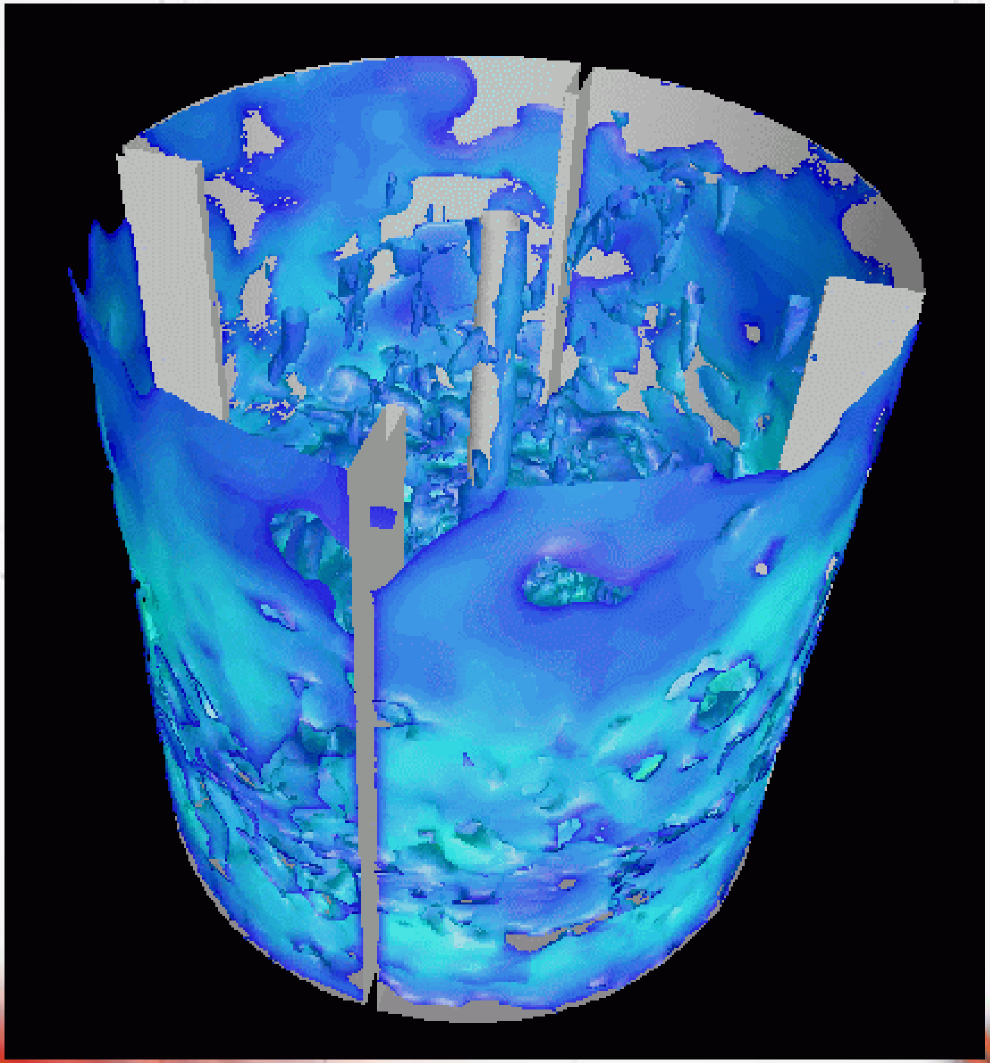
Applications

Mixing Analysis



- CFD Analysis
  - 2 Dimensional
    - Fixed Velocity
  - 3 Dimensional
    - Fixed Velocity
    - MRF
    - Sliding Mesh

Mixers



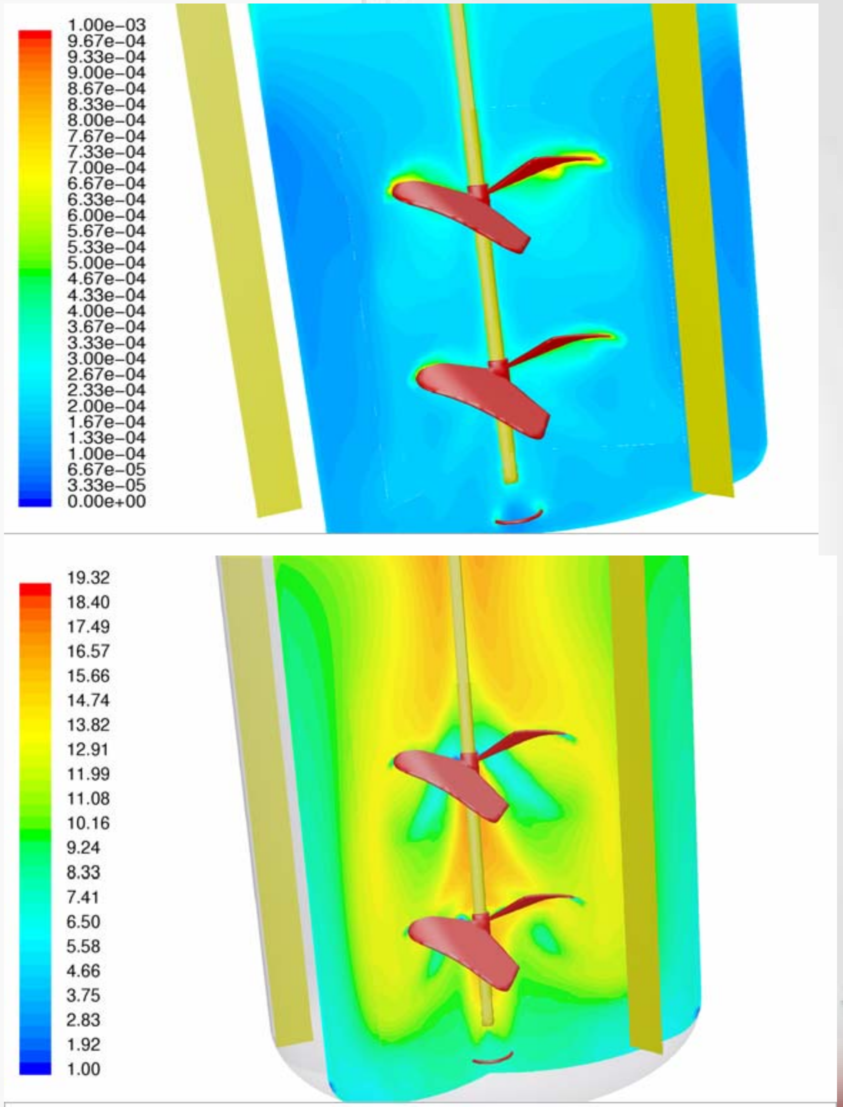
LES Simulation of a Mixing Tank

Gas-Liquid Stirred Tanks

- K_l is obtained

$$K_l = 0.301(\varepsilon \nu)^{0.25}(Sc)^{-0.5}$$

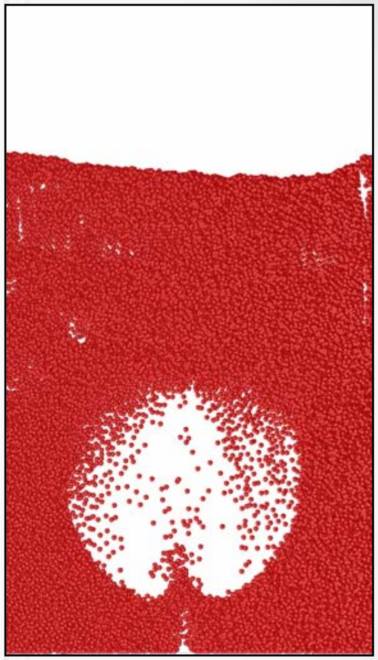
  - From Kawase and Moo-Young, 1990
  - Sc is Schmidt Number
- CFD shows distribution of K_L values and bubble diameter



Contours of Diameter (air) (mm)

FLUENT 6.1 (3d, dp, segregated, eulerian, rke, unsteady)

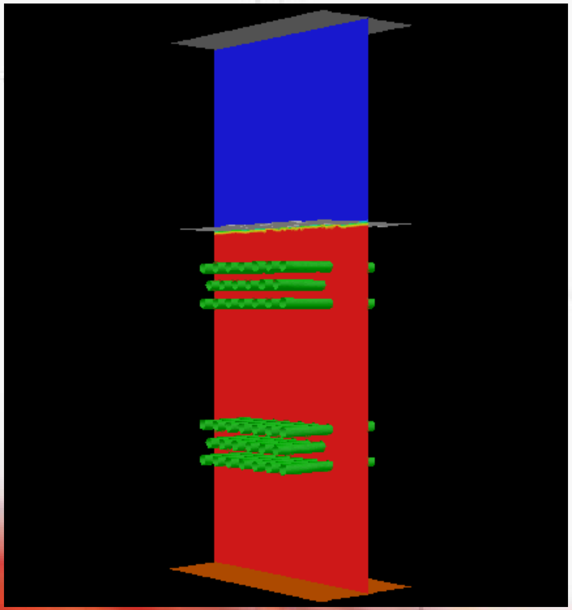
Particle Flows



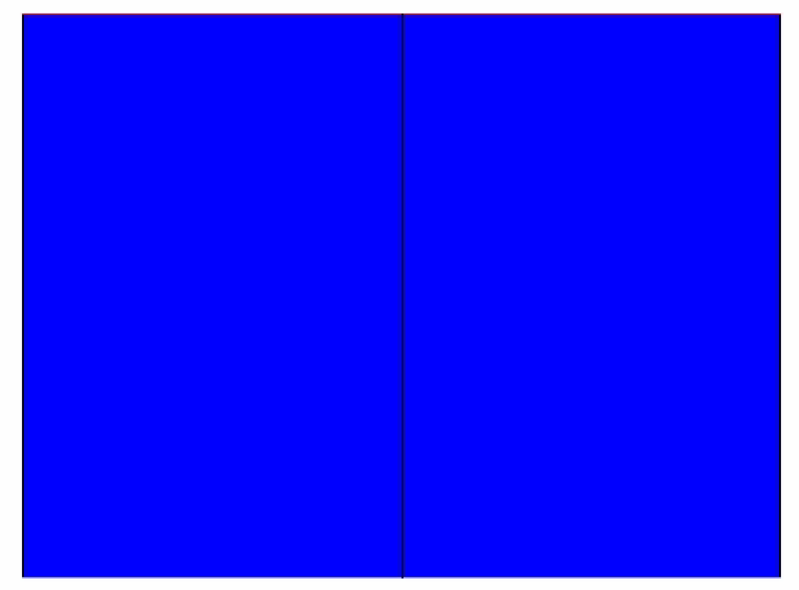
Two Fluid approach: Fluidization

- Euler-Euler or Mixture Model
  - Modifications Include
    - Solids Pressure
    - Solids Shear Stresses (using an effective viscosity term)
    - Granular Temperature calculated using a partial differential equation
    - Heterogeneous mass transfer

Fluidized bed with heat exchanger



Ozone decomposition

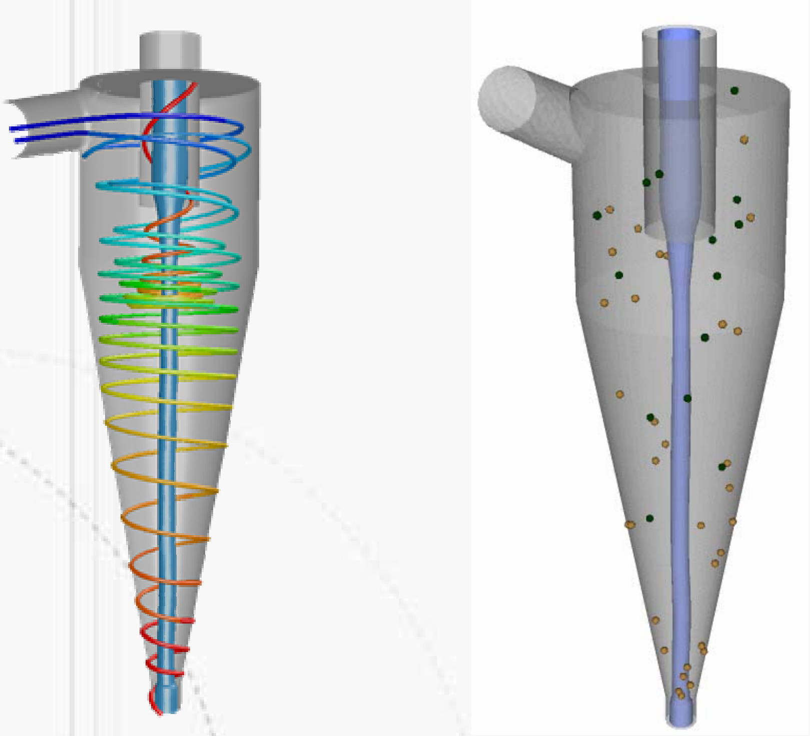


O_3 Mass Fraction in Gas Phase

CREL meeting 2005

Discrete particle model

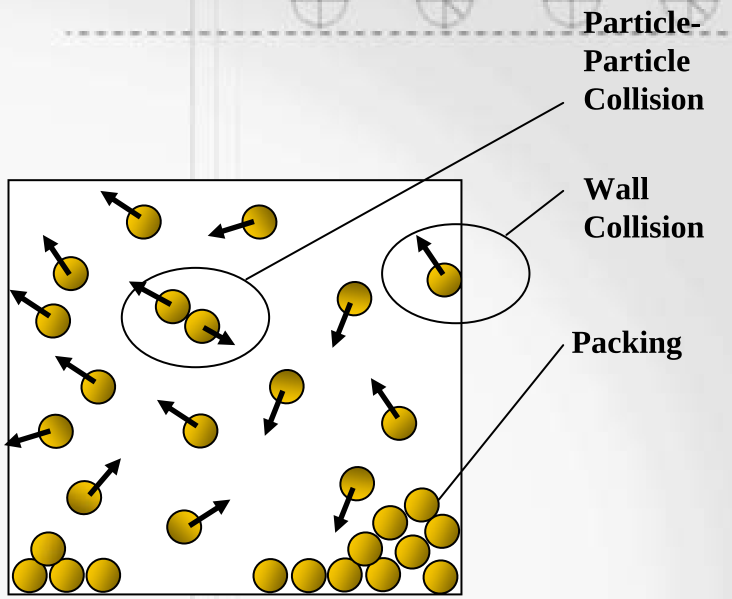
DPM: Particle separation in a hydrocyclone

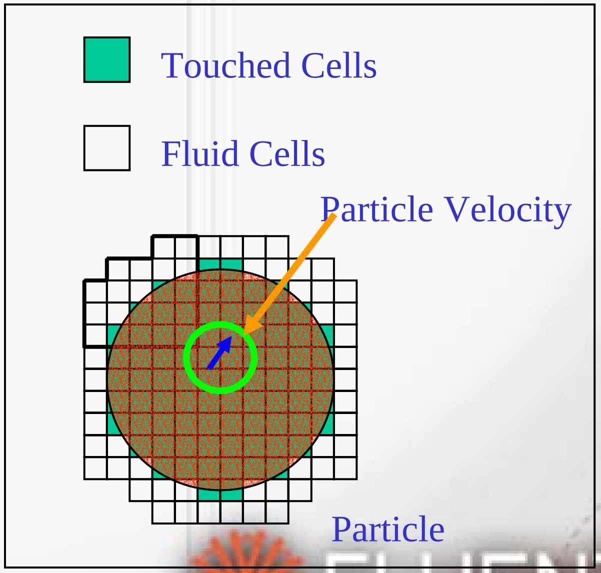


Dark particles are small and less dense
Orange particles are larger and more dense

Macroscopic Particle Model
(Agrawal et al.2004)

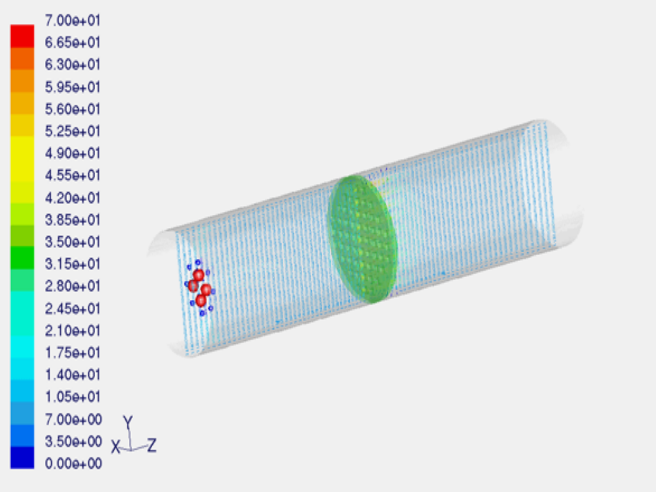
- The particles are modeled in a Lagrangian frame of reference (like DPM)
  - particle to particle collisions
  - particle to wall collisions
- For each particle a “rigid body velocity” is imposed in the cells that represent the particle.
- The presence of the particles requires that there is momentum transfer between the particles and the fluid.
- The integral of the momentum deficit gives the particle drag and the particle torque for each particle.

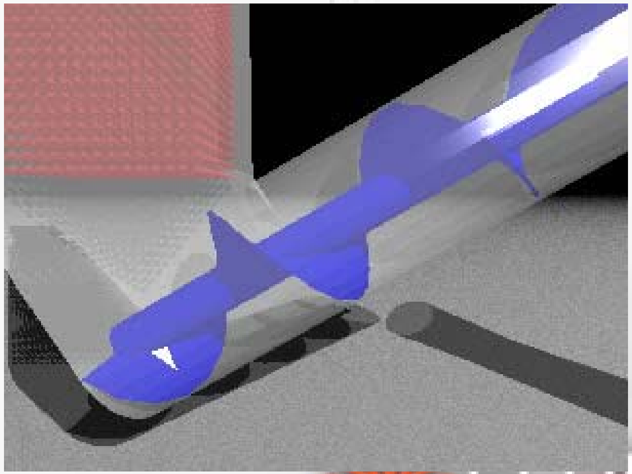




Application of Macroscopic Particle Module

- Ball milling
- Particle-Fluid Separators
- Micro particle separators
- Particle Filters
- Materials Handling
- Drilling
- Fluid-Solid Mixing
- Hoppers
- Blood flow and Biomedical
- Sports

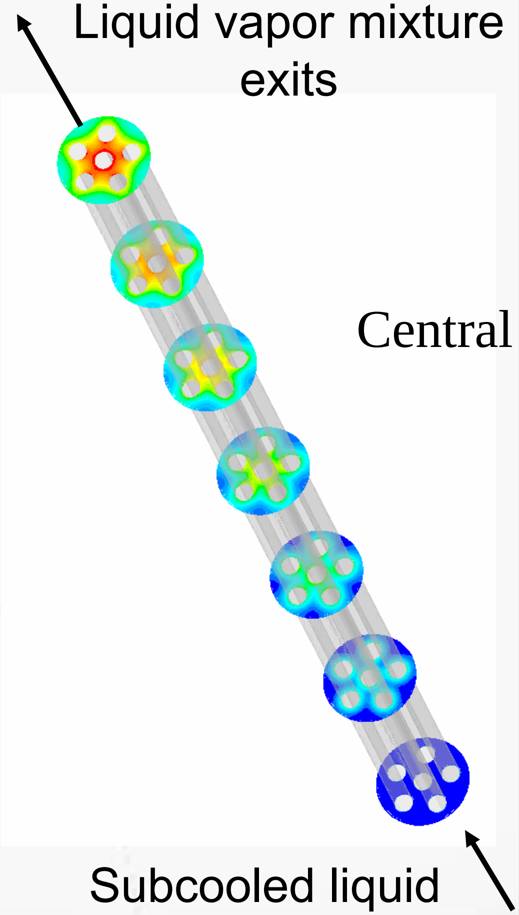




Reactor Core Flows

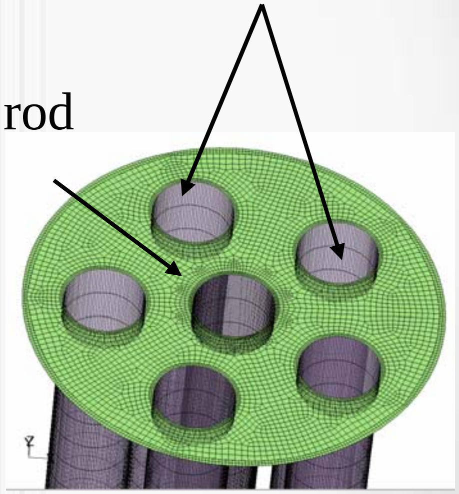
Boiling flow in nuclear reactor

- Flow in nuclear fuel assembly
  - Pressure 50 atm
  - Re_{liq}=300,000
  - Heat flux 0.522 MW/m^2
  - Inlet subcooling 4.5 K
  - y_+=100



Liquid vapor mixture exits

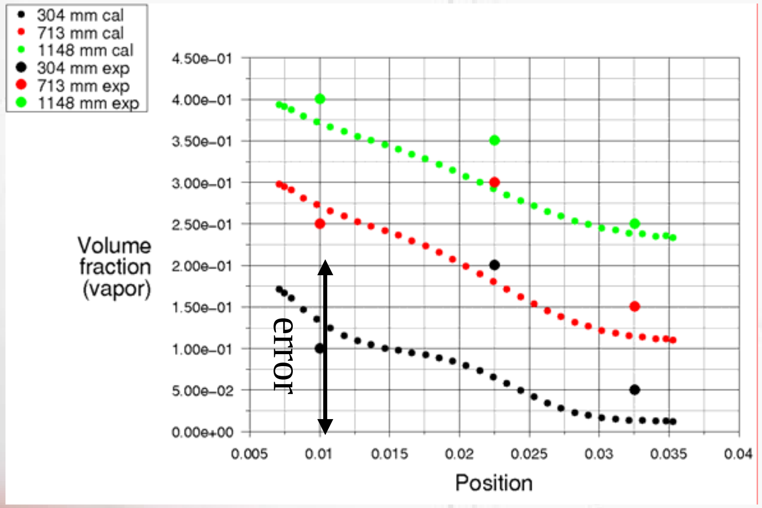
Subcooled liquid enters



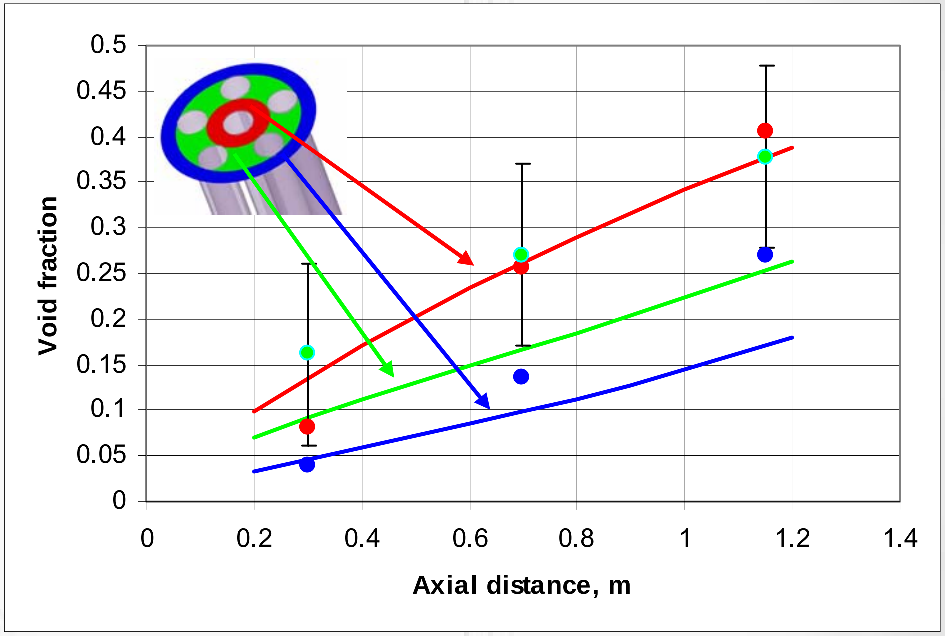
Central rod

Side rods

Boiling flow in nuclear reactor (2)



Comparison with experiment for lateral vapor void fraction

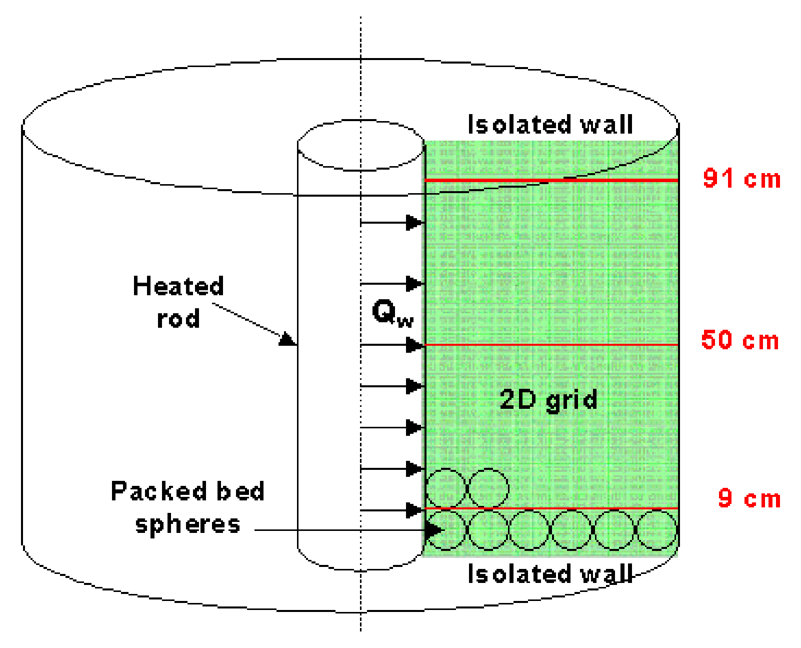


Comparison with experiment for area averaged vapor void fraction for different zones

Gas Cooled Reactors

Pebble Bed Modular Reactor

- The pebble bed modular reactor (PBMR) is a novel nuclear reactor
- The reactor core is an annular packed bed of spheres of fissile material
- The heat-generating spheres are cooled by gas flow in the container
- Experiments on a mock-up facility* have been simulated in FLUENT

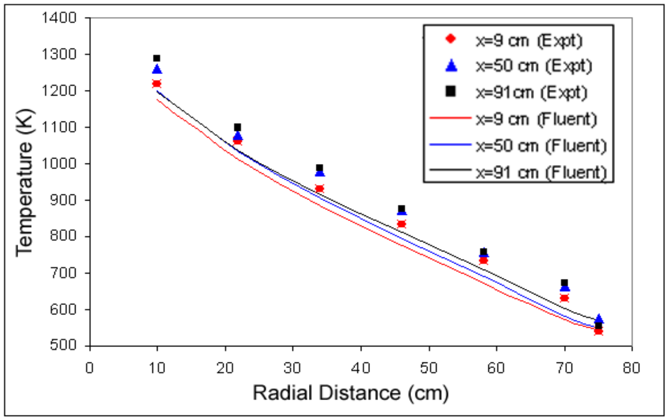


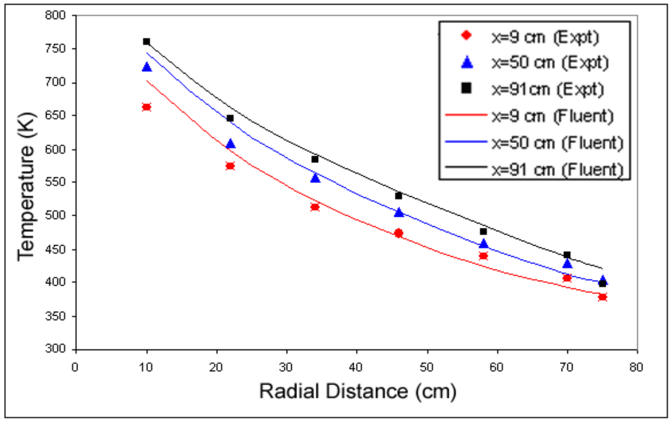
- Post shutdown emergency situation considered
- The packed bed Eulerian multiphase model is used

** B. Stoker, Dissertation RWTH Aachen 1998.*

Pebble Bed Modular Reactor

- Predictions for temperature profiles at 3 axial locations are compared to data **
- The inner container wall heats the annular bed of non-fissile spheres
- Radiation included
- Temperature profiles using helium gas at high (top) and low (heat flux) show little stratification
- This suggests that radiation is an important heat transfer mechanism





*** P. Zehner and E. U. Schlunder, Chemie Ing. Techn.* ***42****(14), 1970.*

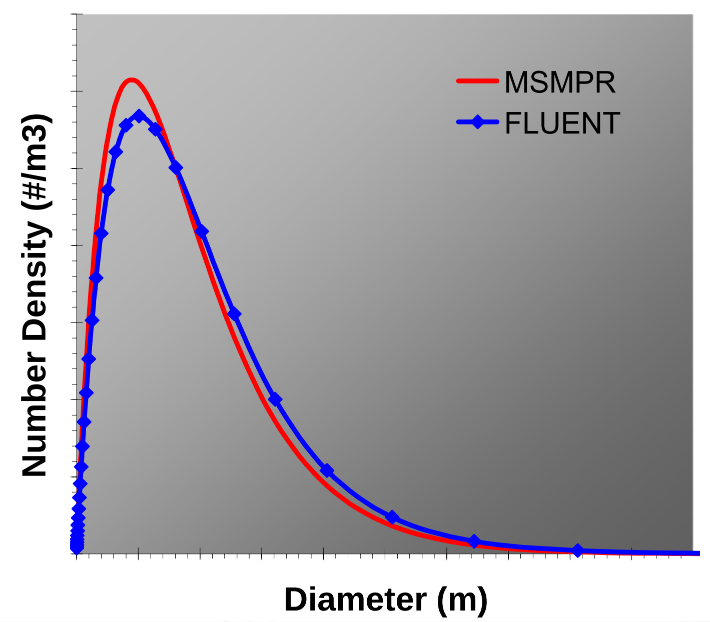
Population Balance Modeling

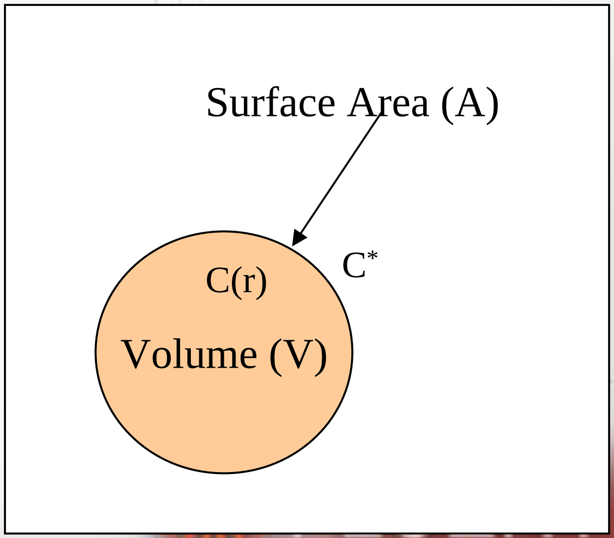
And applications to crystallization and bubble columns

he process industry, many unit operations are performed in
reactors. Thanks to ongoing advances in flow modeling te
iled insight of the flow-dependent processes inside such eq
dily be gained using numerical simulation.

Size Distribution Modeling

- What is size distribution modeling
  - Multiphase problem
  - Secondary phase has a size distribution
- Population balance problems include
  - Aerosols
  - Polymers
  - Solution Crystallization
  - Bubble Columns
  - Gas-Liquid Mixing
  - Bioreactors
- Why is size distribution modeling important
  - Downstream processing
  - Product quality
  - Mass transfer and heat transfer
    - Rate = kA(C-C*)

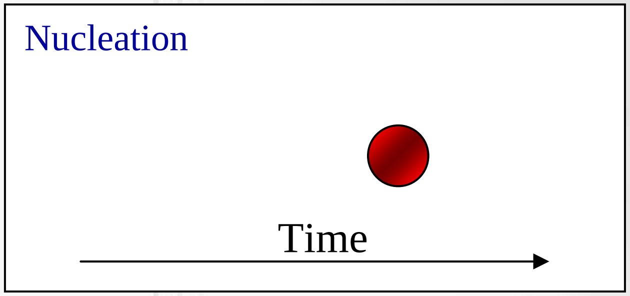


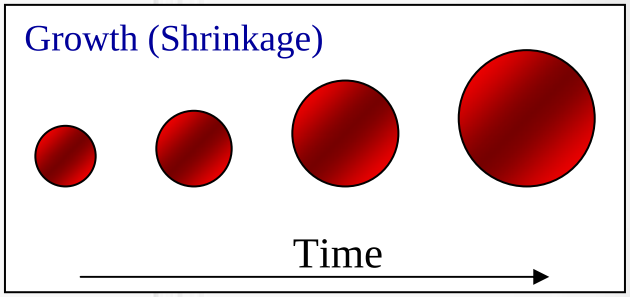


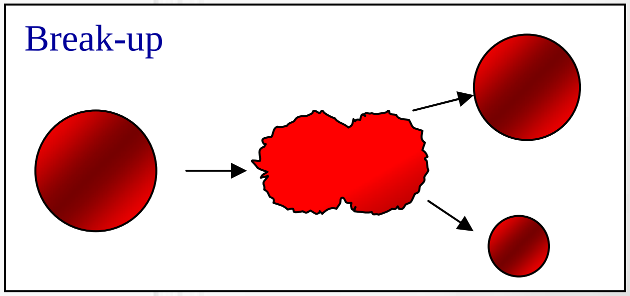
CREL meeting 2005

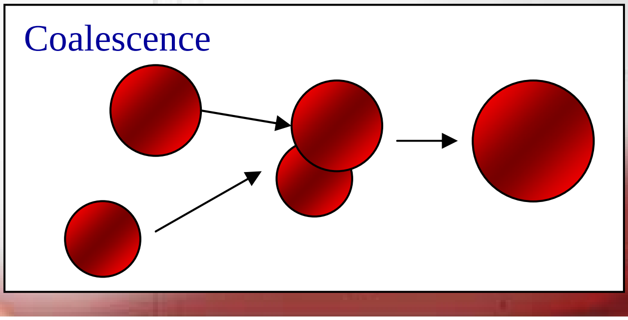
What Influence Secondary Phase Particle Size

- Nucleation
  - Production of new secondary phase particles
- Particle Growth
- Break-up of Particles
  - Particle-particles collisions
  - Hire stresses
- Coalescence of Particles
  - Particles sticking together







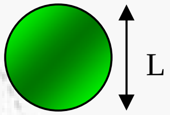


Population Balance Equation (PBE)

- A conservation law can be written for the number density function.

$$\underbrace{\frac{\partial n(V)}{\partial t}}_{\text{Transient Term}} + \underbrace{\nabla.\mathbf{v}n(V)}_{\text{Convective Term}} + \underbrace{\nabla.Gn(V)}_{\text{Growth Term}} = \underbrace{B(V) - D(V)}_{\text{Birth and Death Terms due to Nucleation, Aggregation and Breakage}}$$

$$G = \frac{dV}{dt}$$



$$V = K_v L^3$$

- Growth is rate of change of particle size
  - Physics/ Chemistry based or empirical

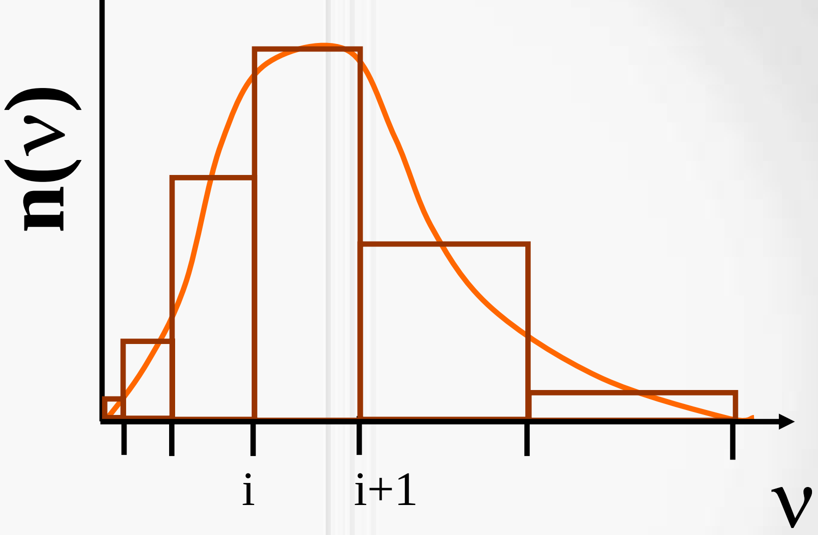
Solution Methods

Discrete Method

- Discretize the particle population into a finite set of size intervals:

$$N_i = \int_{v_i}^{v_{i+1}} n(v; X, t)\,dv$$

$$\frac{v_{i+1}}{v_i} = 2^q$$



- Solve equations for N_i
- Computationally expensive if large number of discrete size intervals are needed.
  - For example in crystallization, nucleation may occur in microns or nanoscales, but growth and aggregation can create particles in mm

Solution Methods (cont)

Method of Moments

- Standard Method of Moments (SMM):
  - Only size-independent or linear growth allowed
  - Constant Aggregation Kernel
- Quadrature Method of Moments (QMOM)
  - Overcomes the limitations of the standard closure.
  - All the integral terms are solved by constructing a quadrature approximation

$$n(L;t) \approx \sum_{i=1}^{N_q} w_i(t)\,\delta\big(L - L_i(t)\big)$$

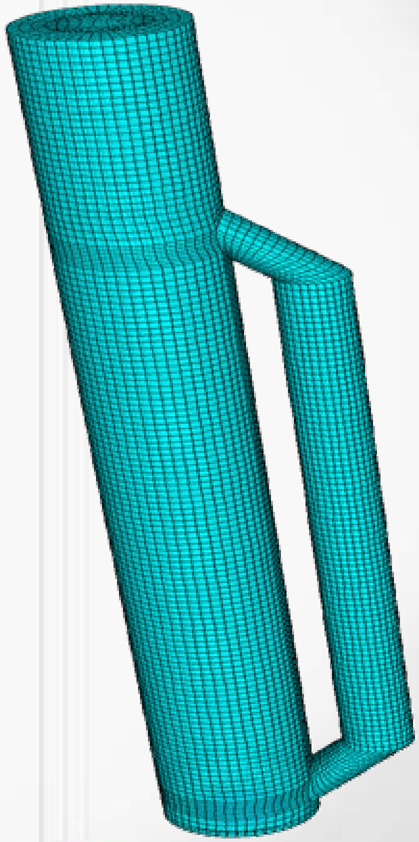
$$m_k(t) \approx \sum_{i=1}^{N_q} w_i(t)\,L_i^k(t)$$

  - No limitations on nucleation, growth, aggregation or breakage kernels

Bubble Columns

Bubble Columns Gas-Liquid Mixing

- Eulerian-Eulerian 2 phase simulation
  - Gas hold-up
  - Mass Transfer
    - Need bubble size distribution to predict the specific surface area
    - Need to estimate the mass transfer coefficient
  - Other considerations
    - No nucleation
    - No growth terms
    - Break-up based on the local turbulence field
    - Collision based on kinetic gas theory

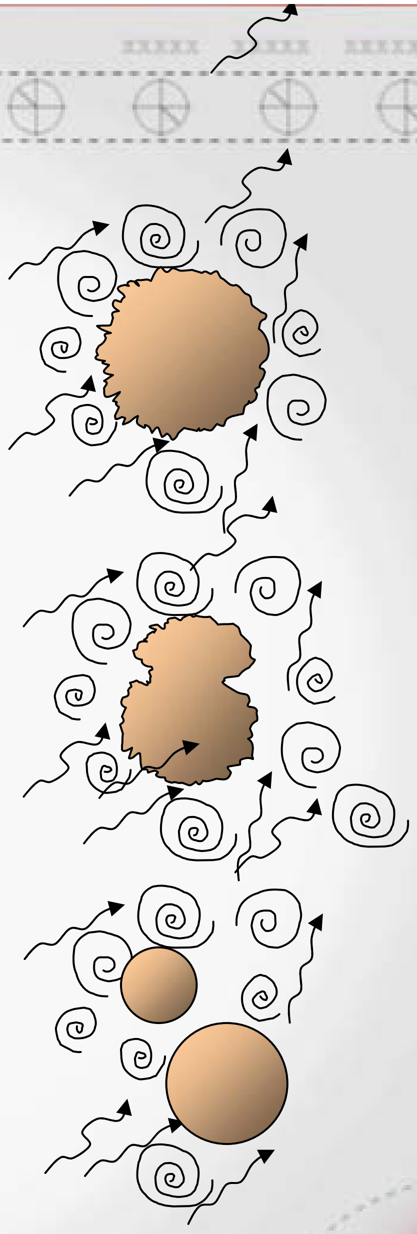


CREL meeting 2005

Bubble Breakup (Luo, 1993)

- Bubble breakup is assumed to be caused by bubble **interactions** with **turbulent eddies**.
- Breakup occurs if the increase in surface energy due to deformation is beyond a critical value.
- The model contains **no adjustable parameters**.
- The breakup rate of particles of size ν into particle sizes of $\nu \cdot f_{BV}$ and $\nu\,(1-f_{BV})$ is given as:

$$\frac{\Omega_B(v : vf_{BV})}{(1-\varepsilon_d)n} = c_4\left(\frac{\varepsilon}{d^2}\right)^{1/3}\int_{\xi_{\min}}^{1}\frac{(1+\xi)^2}{\xi^{11/3}}\exp\left(-\frac{12\,c_f\sigma}{\beta\rho_L\varepsilon^{2/3}d^{5/3}\xi^{11/3}}\right)d\xi$$



*H. Luo. Ph.D. Thesis. Department of Chemical Engineering, Trondheim, Norway (1993).

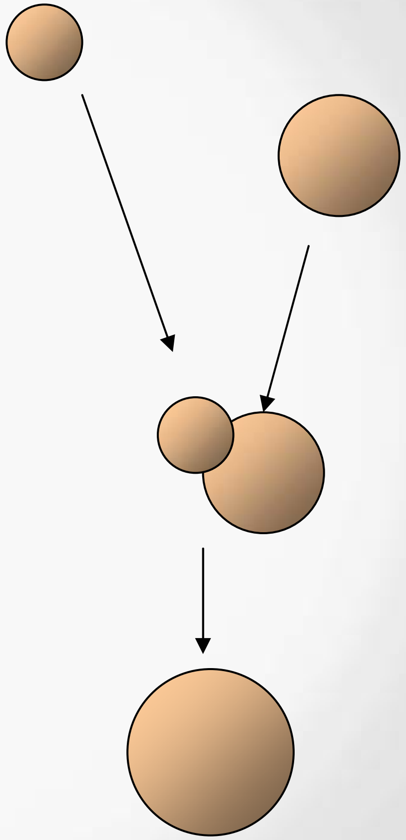
Coalescence

- Bubble **coalescence** is modeled by considering bubble **collisions** due to turbulence, buoyancy and laminar shear.
- The model is a combination of **collision frequency** and **coalescence probability**.
- The **coalescence probability** of particles of sizes u_i and u_j is expressed as:

$$P_C(v_i,v_j) = \exp\left(-c_1\rho_L d_i (u_i^2+u_j^2)^{1/2} \frac{[0.75(1+\xi_{ij}^2)(1+\xi_{ij}^3)]^{1/2}}{\sigma(\rho_G/\rho_L+\gamma)^{1/2}(1+\xi_{ij})^3}\right)$$

- The **collision frequency** is based on **kinetic gas theory**:

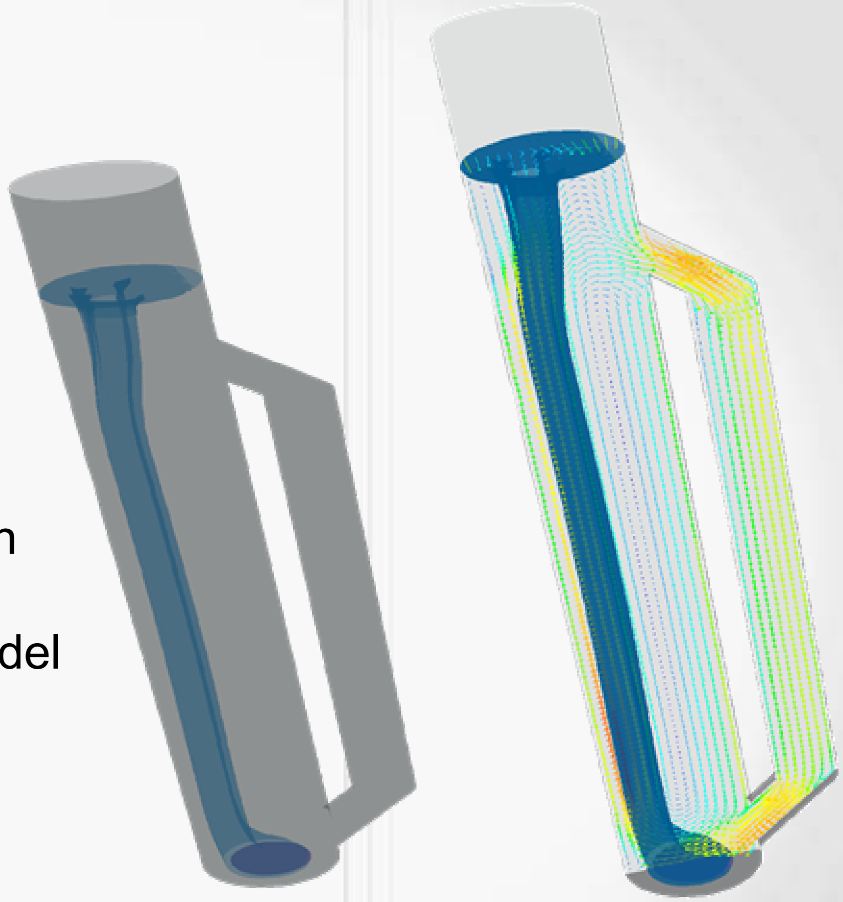
$$\omega_c(v_i,v_j) = (\pi/4)(d_i+d_j)^2 n_i n_j (u_i^2+u_j^2)^{1/2}$$



Results on a bioreactor

- K_L is obtained from the basis of Higbie's penetration theory as:

$$K_L = \frac{2}{\sqrt{\pi}}\sqrt{D}\left\{\frac{\varepsilon_L \rho_L}{\mu_L}\right\}^{0.25}$$

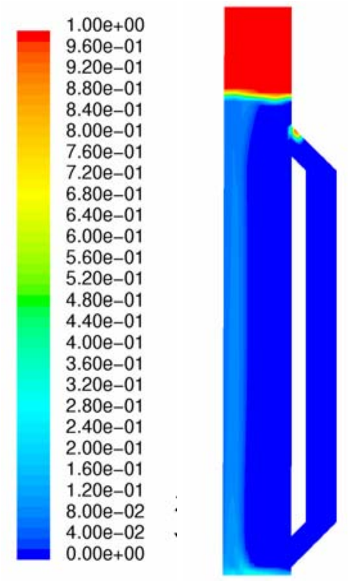


- ε_L (cont. phase turbulent dissipation rate):
  predicted from CFD turbulence model
- The interfacial area a is obtained from the predicted bubble size distribution as:

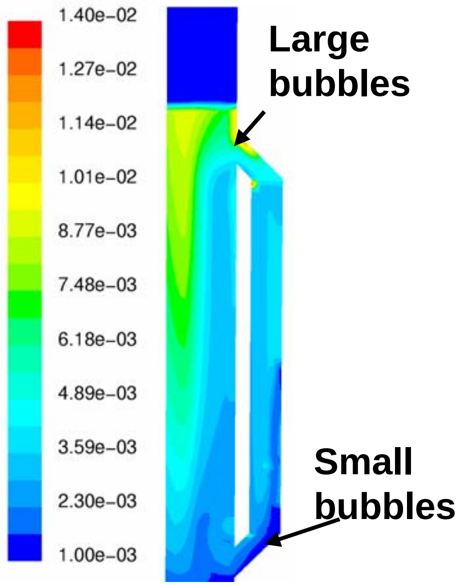
$$a = \sum_i \frac{6\alpha_i}{d_i} \quad \text{(Total Sauter mean diam.)}$$

- $K_L a = 0.037\ s^{-1}$ for air superficial velocity of 0.02 m/s

Bioreactor Results



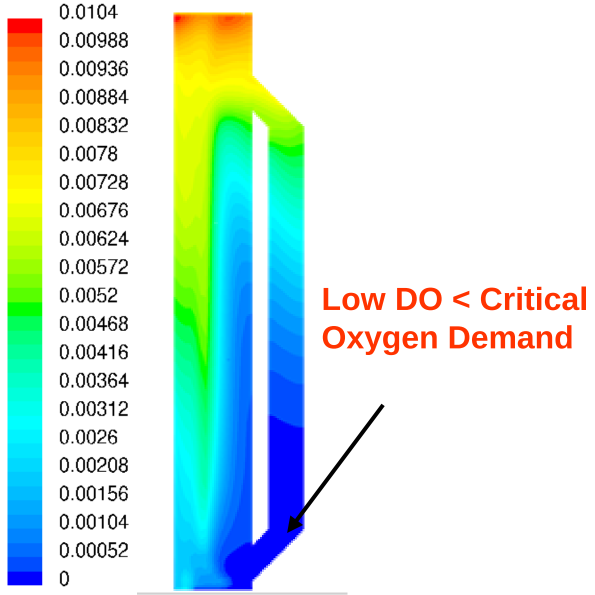
Gas holdup



Large bubbles

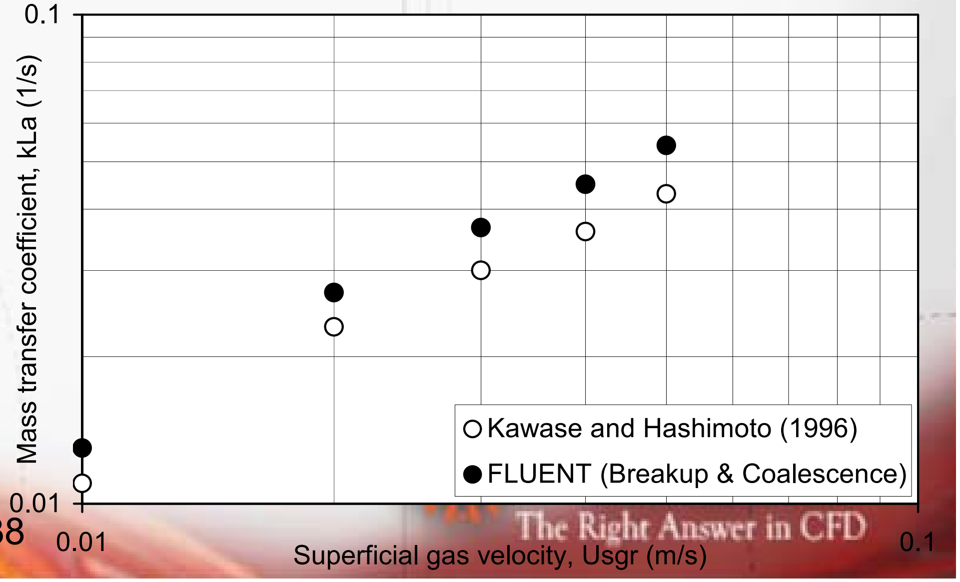
Small bubbles

Sauter mean diameter

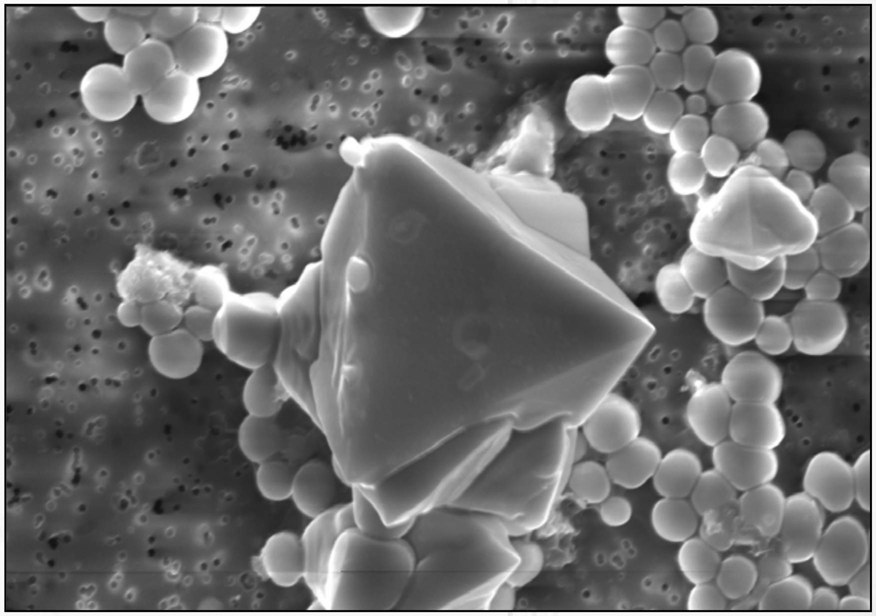


Low DO < Critical Oxygen Demand

Dissolved Oxygen



Application of PBE in modeling Crystallization



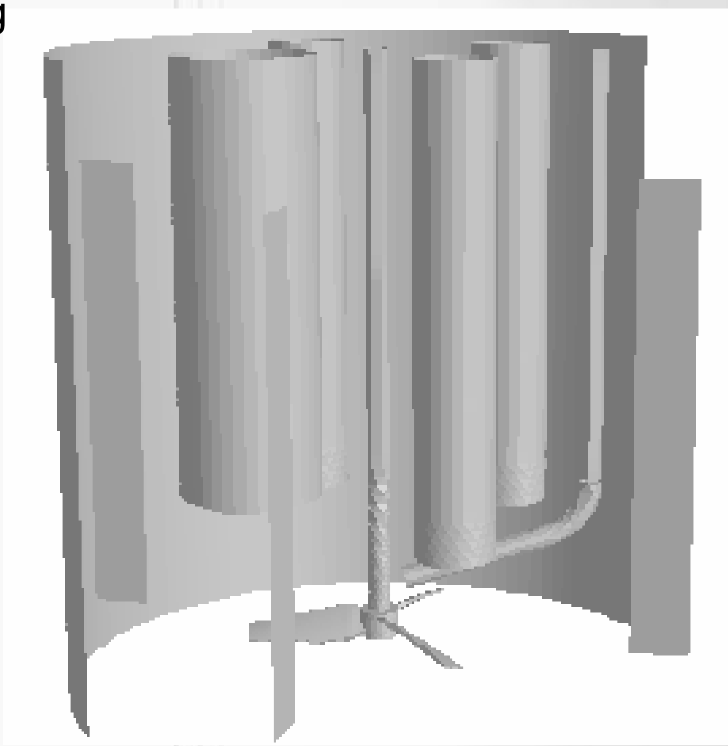
CREL meeting 2005

FLUENT
The Right Answer in CFD

Dow Luddington Pilot Crystallizer

(Courtesy of Dow Chemical)

- Solution of $CaCl_2$, KCl and NaCl from feed entering crystallizer
  - Primary phase consists of mixture of species
- Objective is to enrich KCl and CaCl2 in solution by separation of NaCl (impurity)
- Cooling Crystallization
  - Cooled from 65 to 30-40 C^o in the crystallizer with jacketed wall
  - Saturated feed solution with NaCl solids at 122 microns
- Modeling Approach:
  - Eulerian multiphase with species transport
  - Quadrature Method of Moments
  - 3D with ~ 500,000 cells



Crystallization Kinetics

(Experimental work of Prof. Terry Ring, University of Utah)

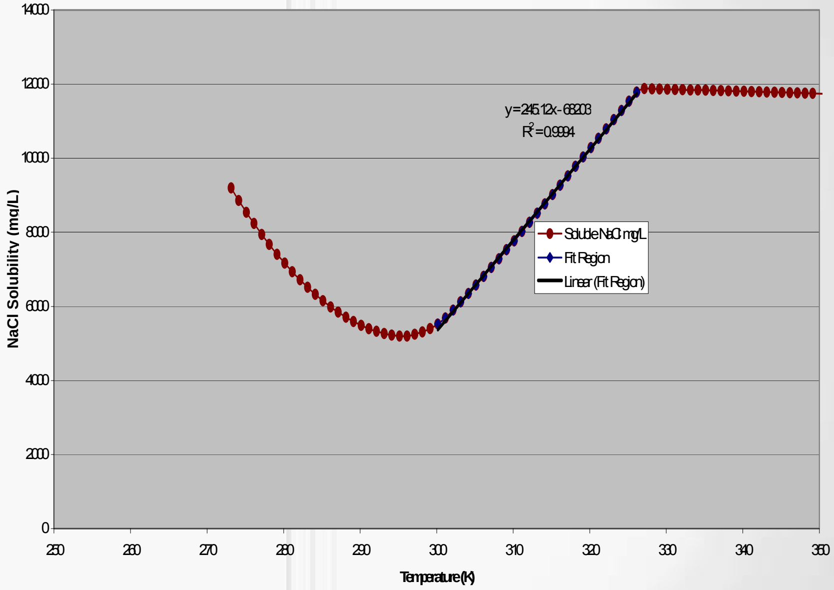
- **Nucleation**
  - Secondary nucleation was assumed to be the dominant mechanism:

$$B^o = 1.824e3 * M_T * (S-1) * (rpm)^2$$

  - Nucleation was applied only near the impeller region
- **Growth**
  - Diffusion limited growth rate was assumed:

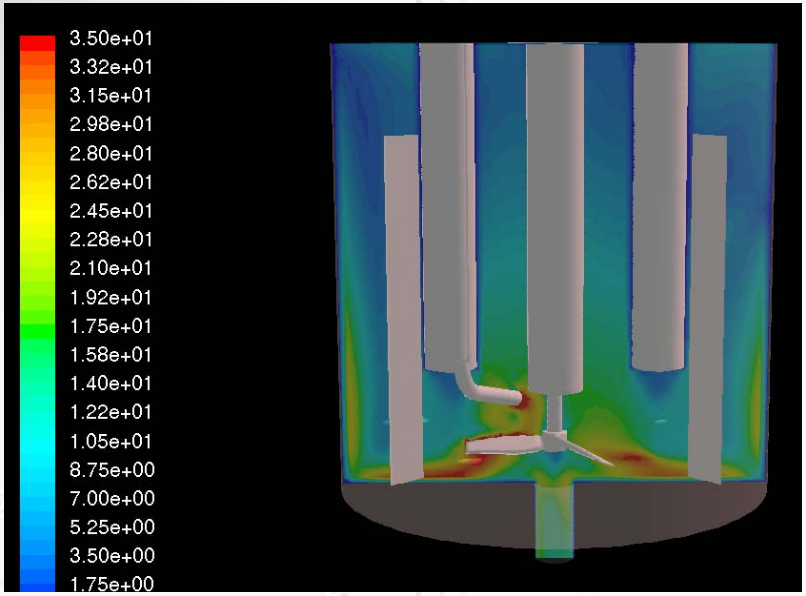
$$G = \hat{V} D C_{eq} (S-1)/l$$

- The kinetics depend on local values of supersaturation ratios in the crystallizer

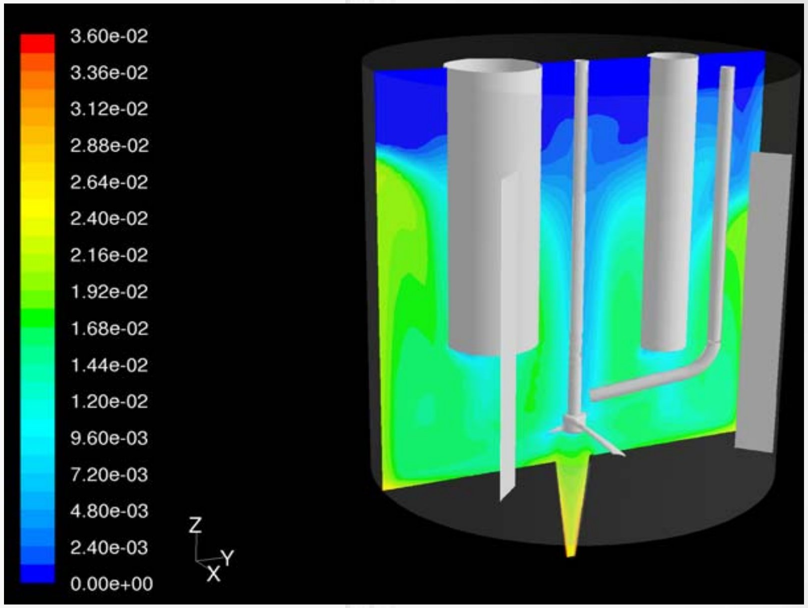


Solubility Curve of NaCl, KCl and $CaCl_2$ mixture

Results



Contours of solution velocity (m/s)

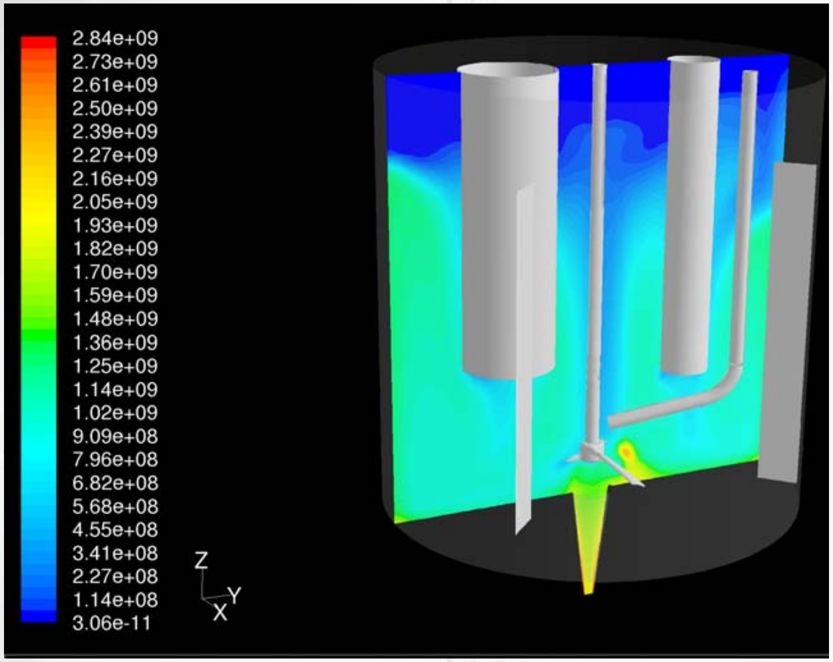


Contours of NaCl(s) volume fraction

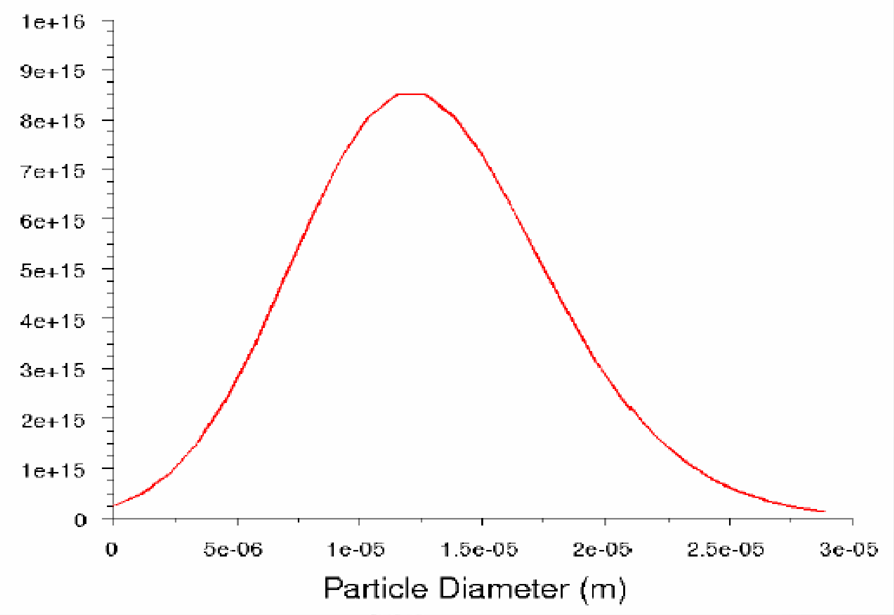
- VOF in regions reaching 3.6%
- At the outlet,
  - the amount of solids is 3%

FLUENT
The Right Answer in CFD

Results (2)



Contours of total number of crystals per unit volume (0th moment)



Crystal number density the outlet

- Distribution of total number density is similar to solids distribution

•The average particle size is 133.8 microns (inlet is 122 microns)

FLUENT
The Right Answer in CFD

Recap

- Various approaches are available in modeling multiphase flows depending of the flow and the regime of interest
- An overview of selected recent application of CFD in the process industries was presented
- To account for particle size distribution solution mythology for population balance equation was reviewed and applications in gas-liquid bio-reactor and a crystallizer were demonstrated