MODELLING OF DENSE GAS-PARTICLE FLOWS USING KINETIC THEORY OF GRANULAR FLOW

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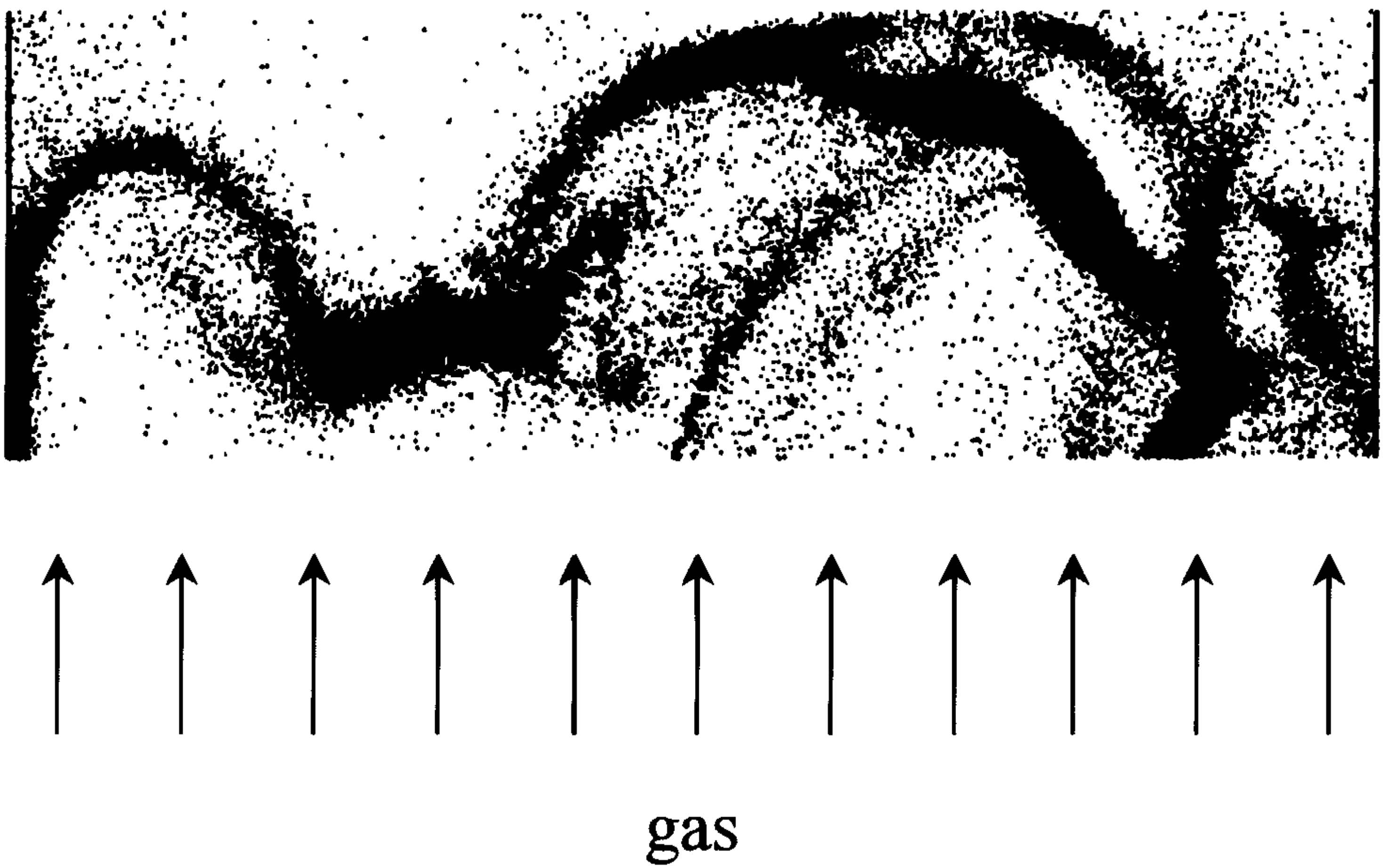
DENSE GAS-SOLID FLOWS

"shifting sands" (Tanzania)

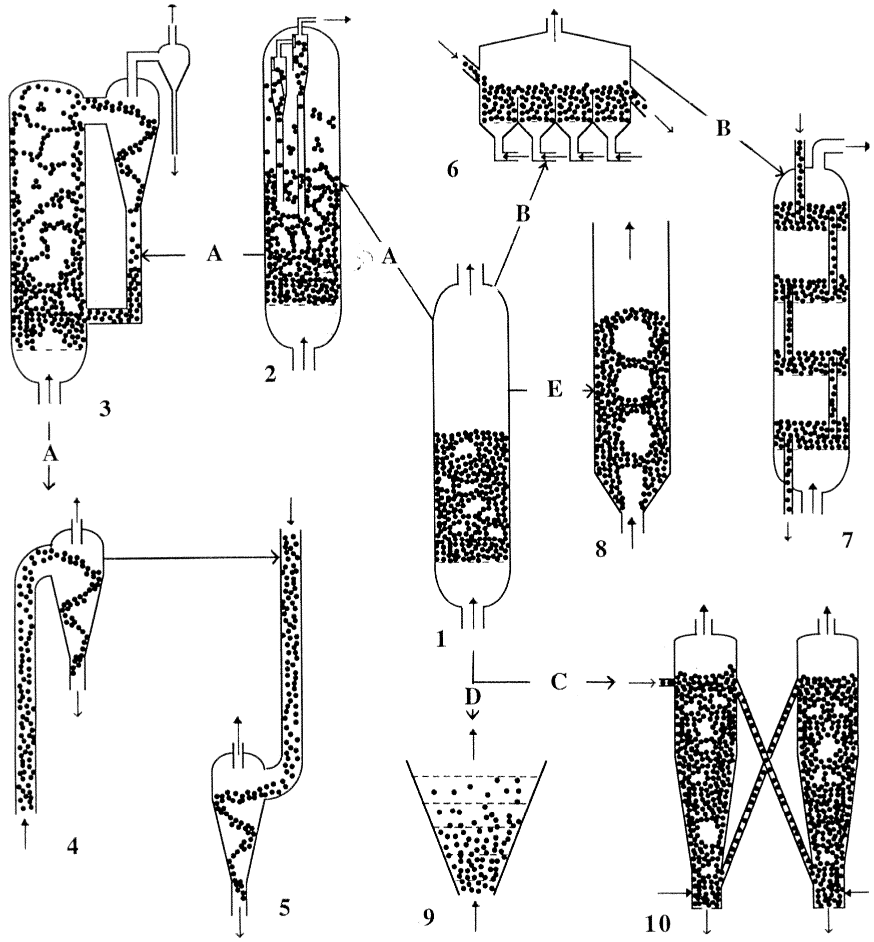
DENSE GAS-SOLID FLOWS

clusters in co-current vertical gas-solid flows



INTRODUCTION

dense gas-particle flows in fluid bed family of contactors



1: bubbling bed
2: turbulent bed
3: circulating bed
4: riser
5: downer
6: lateral staged bed
7: vertical staged bed
8: spouted bed
9: floating bed
10: twin bed

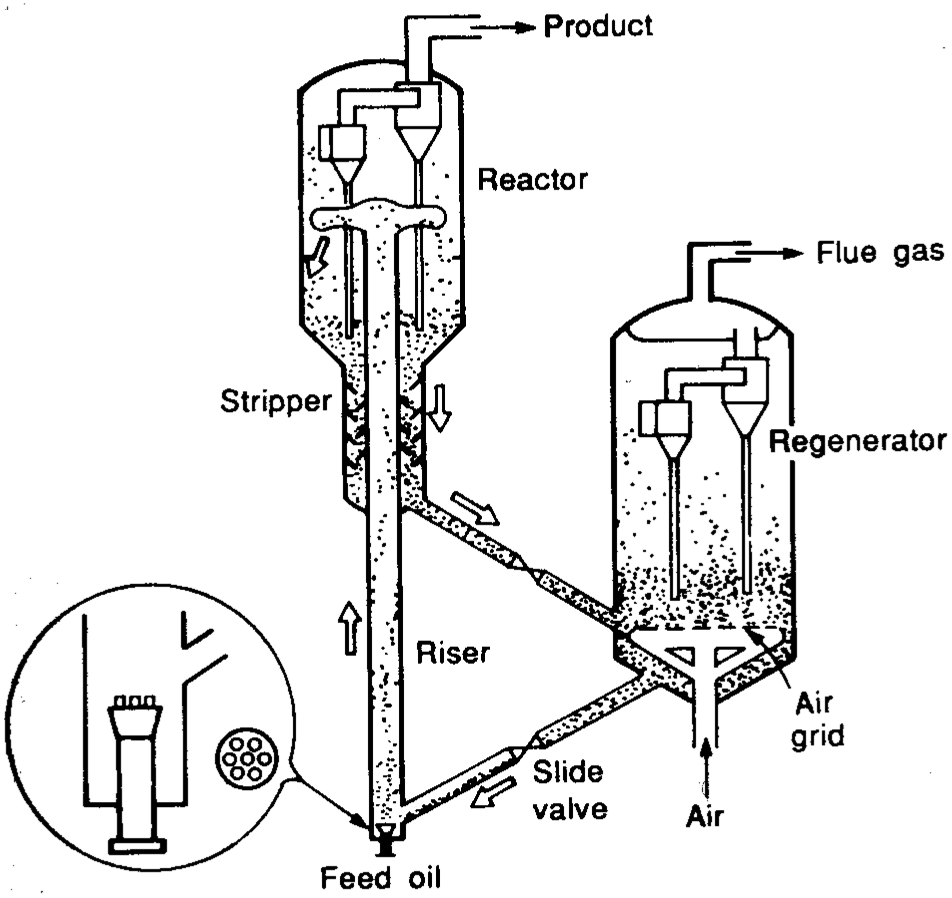
INTRODUCTION

- APPLICATIONS OF FLUIDIZED SYSTEMS

  + heat exchange and drying
  + coating and granulation
  + gas purification via adsorption
  + chemical synthesis (acrylonitrile, maleic and phtalic anhydride)
  + polymerization of lower olefines (propylene)
  + Fischer-Tropsch synthesis
  + Fluid Coking and Flexi-Coking
  + combustion and incineration
  + Fluid Catalytic Cracking (FCC)

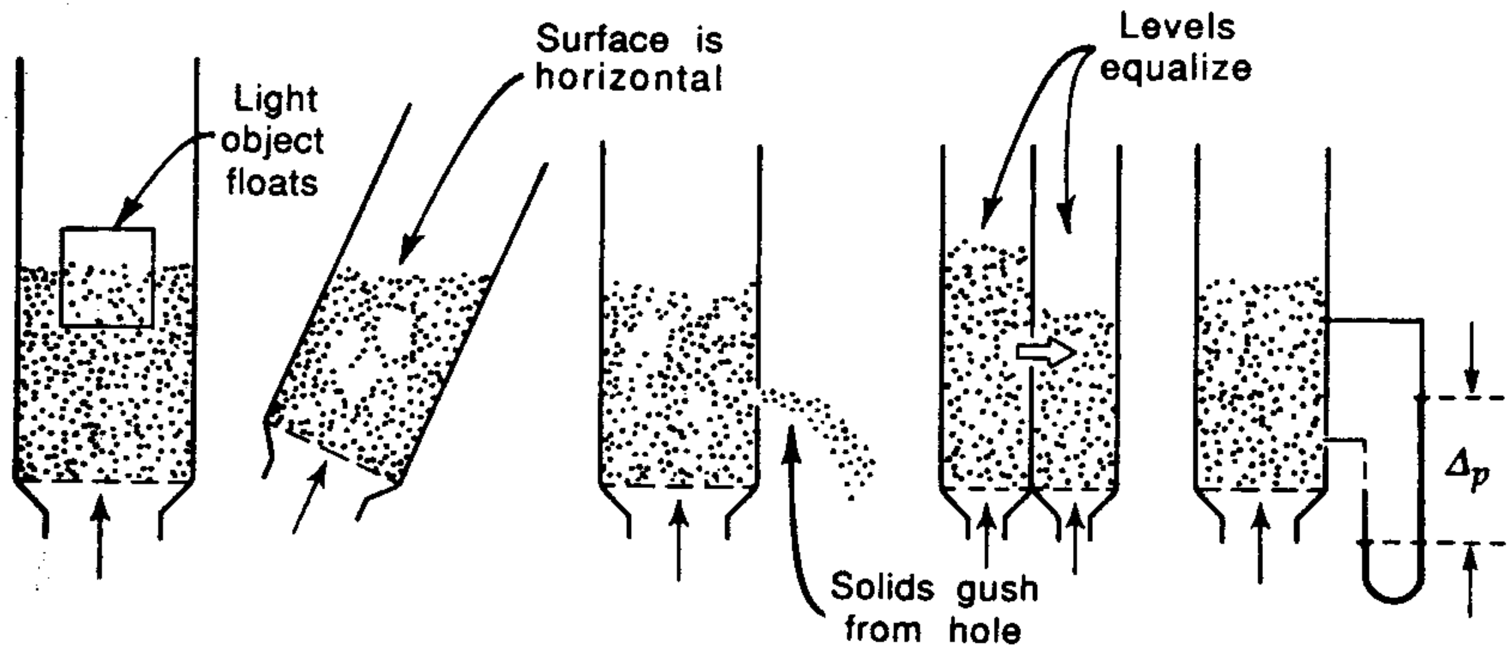
INTRODUCTION

Fluid Catalytic Cracking (FCC) unit



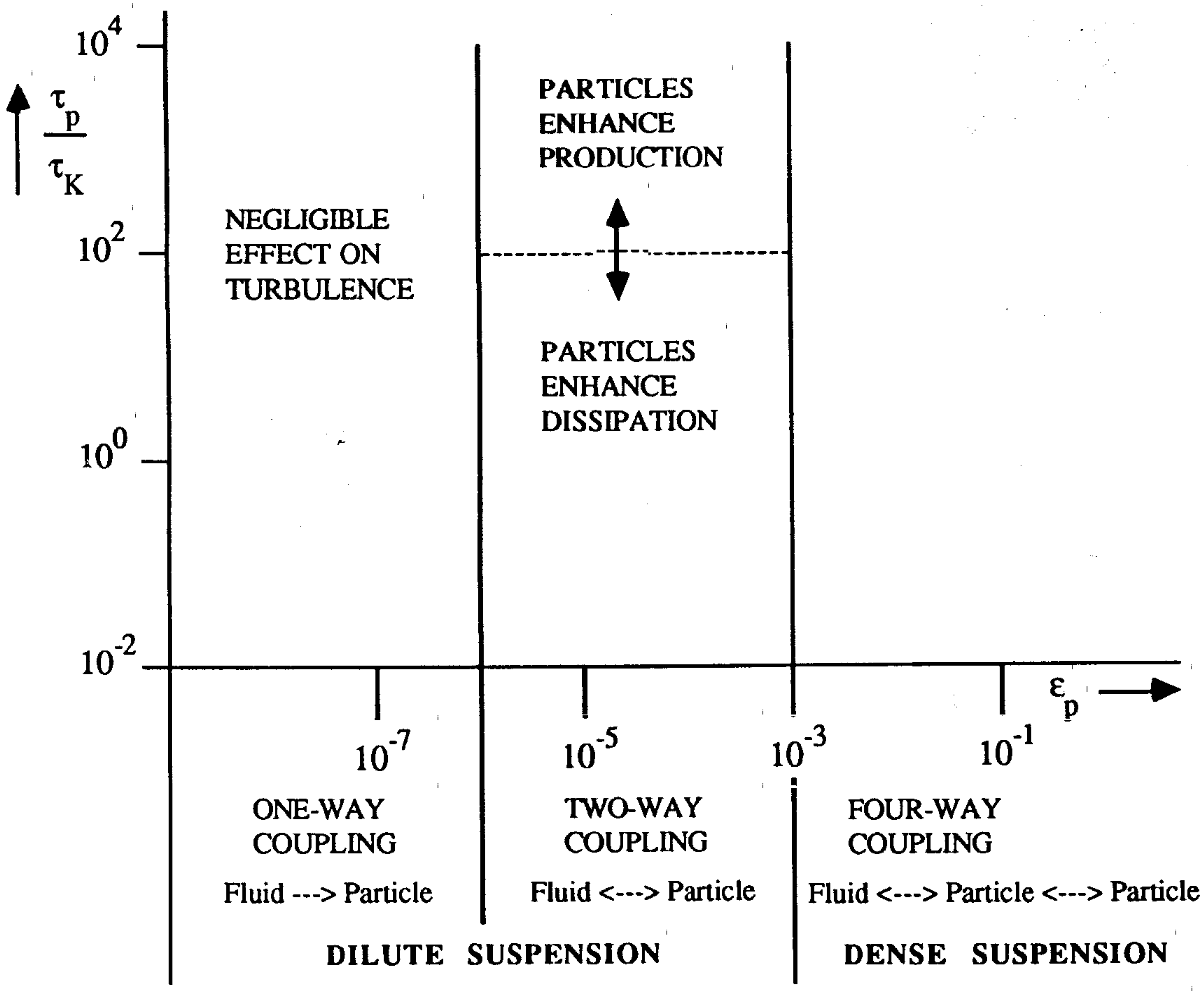
ELEMENTARY PROPERTIES OF GAS-FLUIDIZED BEDS

dense beds



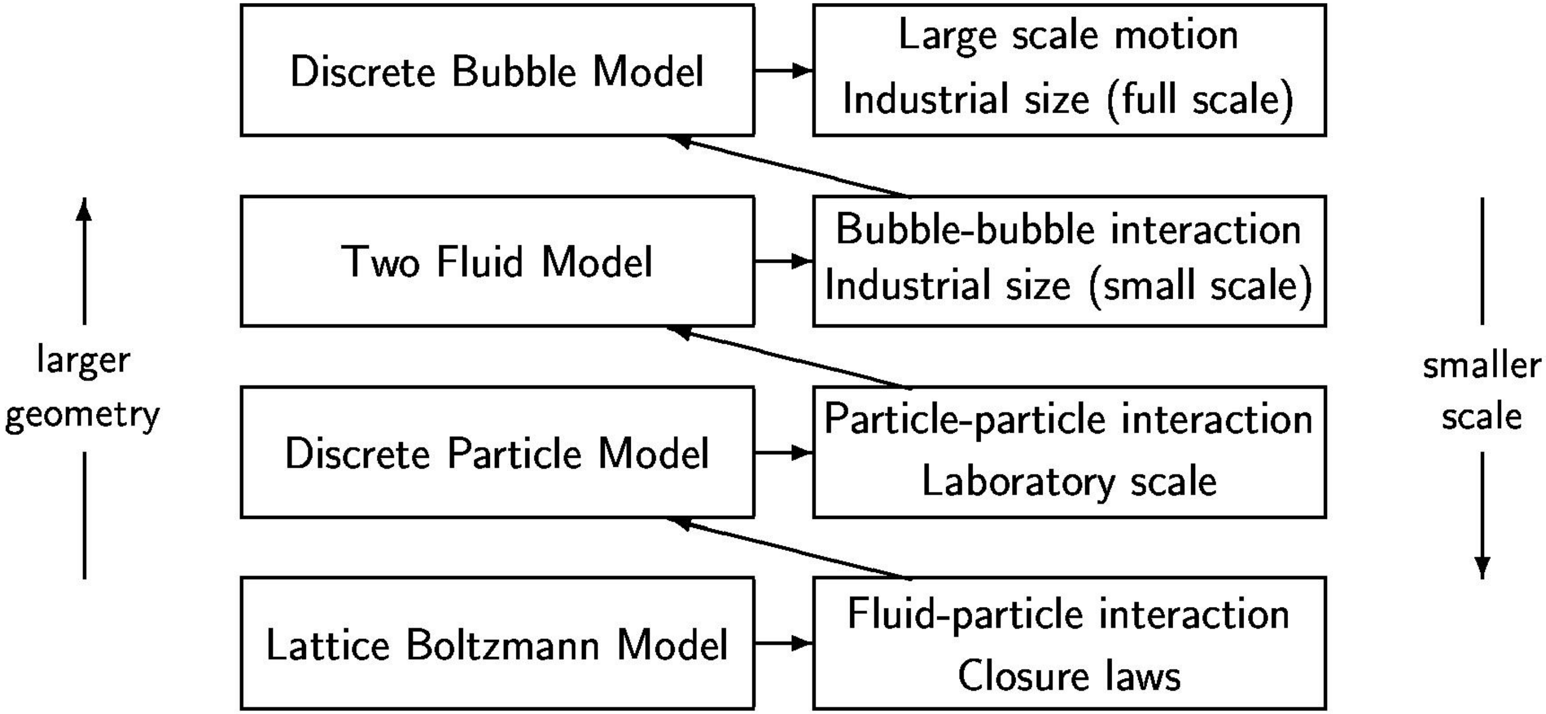
FLOW REGIMES + KEY PHENOMENA

map of flow regimes in particle-laden flows



MULTI LEVEL MODELLING

- MULTI LEVEL MODELLING OF DENSE GAS-SOLID FLOWS



Van der Hoef et al., CES (2004)

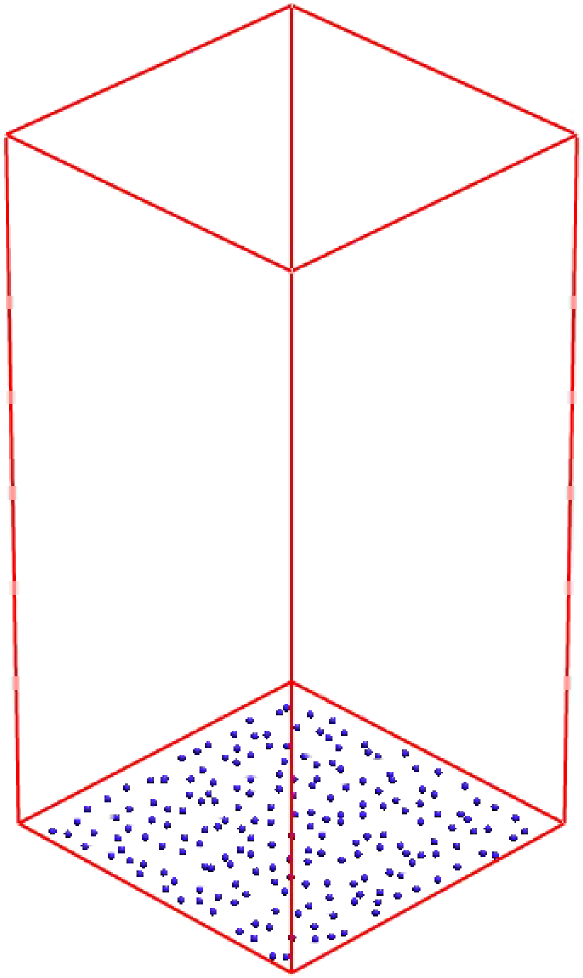
DBM SIMULATION
industrial size column

- SIMULATION CONDITIONS

Industrial scale column:
- Dimensions: 4 m x 4 m x 8 m
- Gas velocity: $2.5U_{mf}$=0.25 m/s

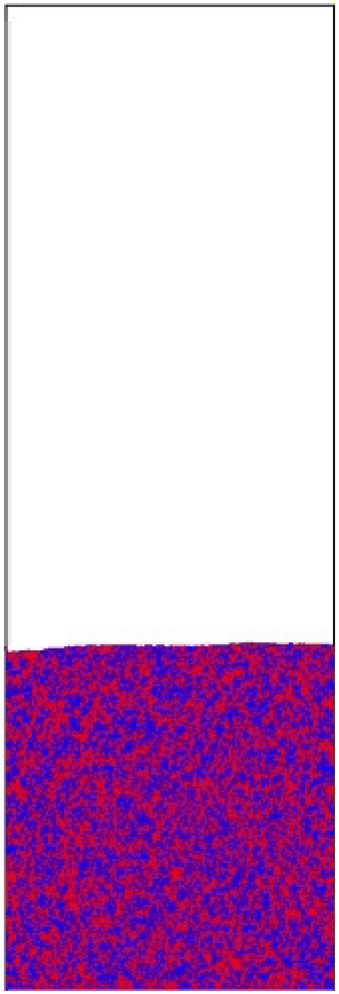
Emulsion phase properties:
- Density: 400 kg/m^3
- Viscosity: 0.1 Pa.s

Bubble properties:
- Initial bubble size: 8 cm
- Maximum bubble size: 80 cm
- Typically ~ 5000 bubbles



DPM + KTGF SIMULATION

bubble formation: 15 cm bed



W=0.15 m

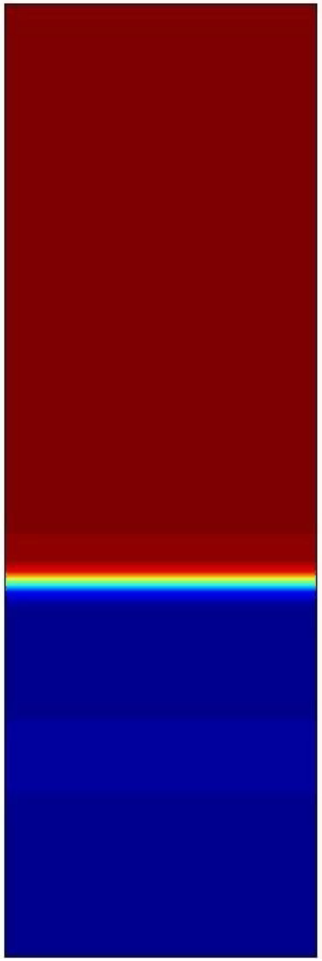
d_p=1.5 mm

ρ_s=2526 kg/m^3

U_b=0.85 m/s

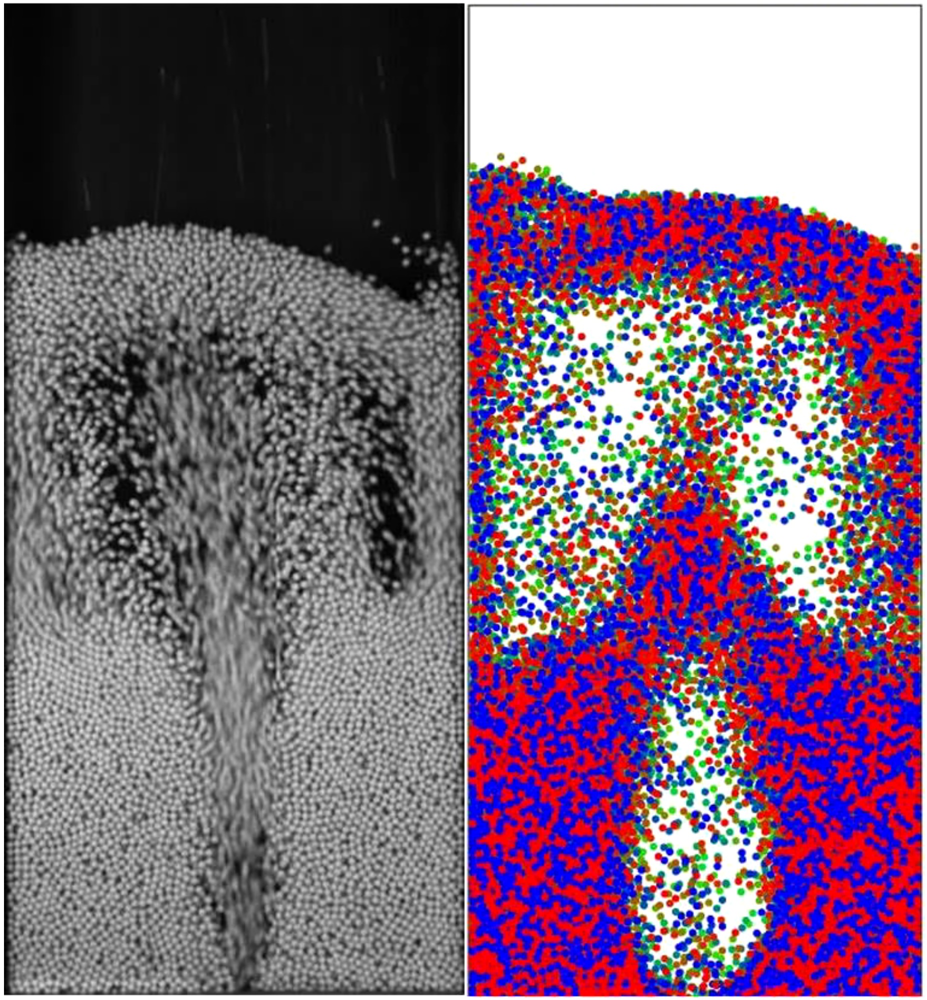
U_j=15.0 m/s

N_p=120000



DPM SIMULATION

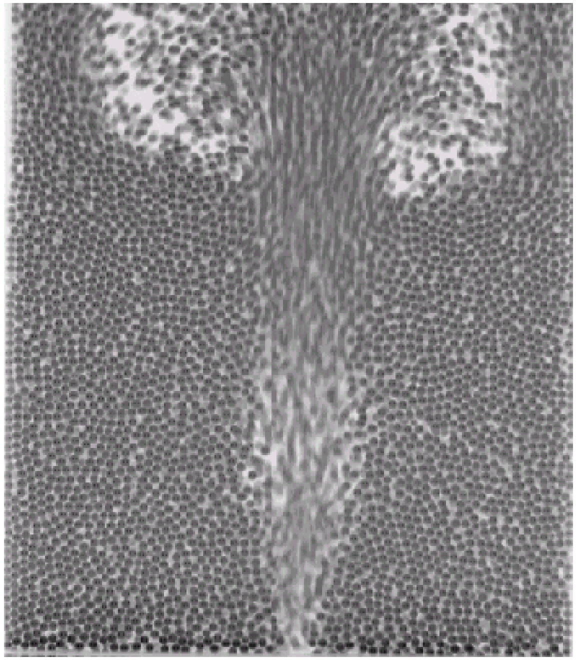
spouted bed

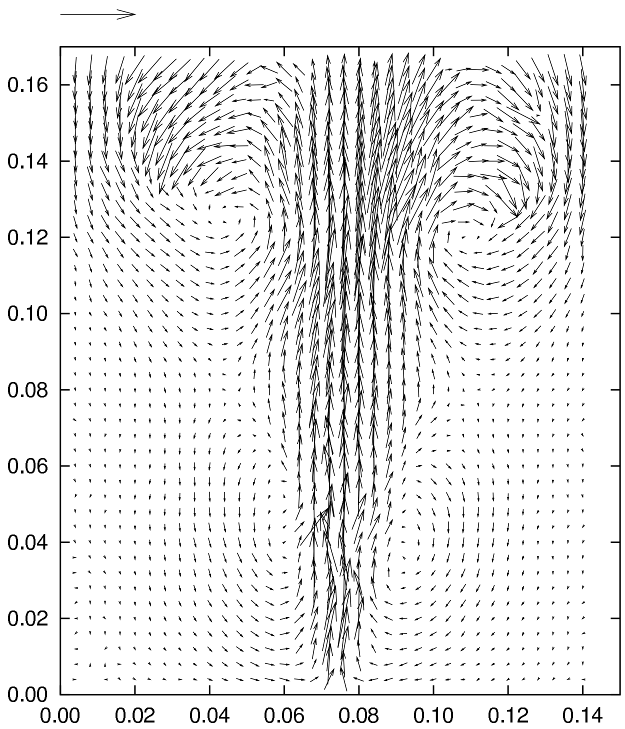


DPM SIMULATION

spouted bed

$$u_{sf}\,/\,u_{mf} = 16.0 \leftrightarrow u_{bf}\,/\,u_{mf} = 1.2$$





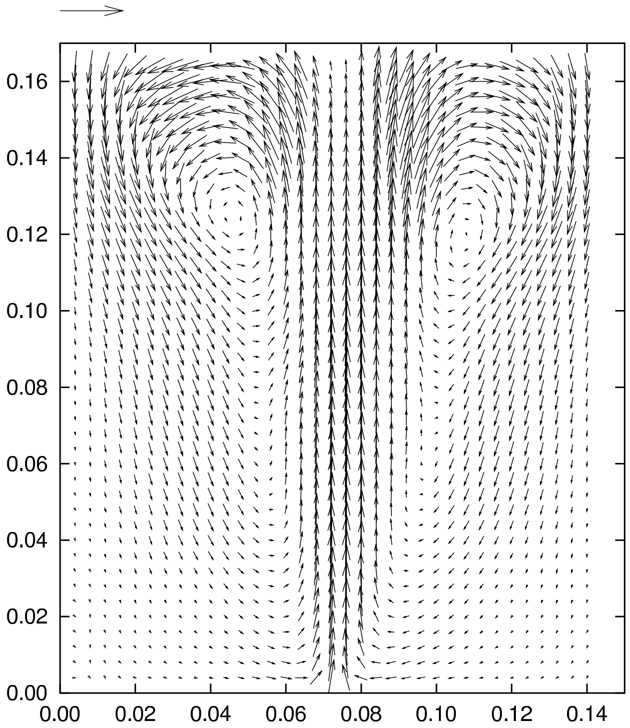
particle configuration

particle velocity map

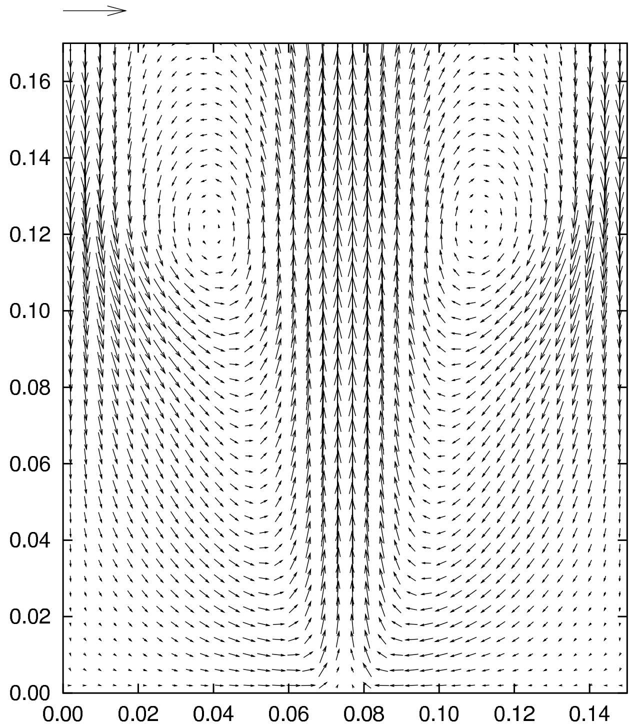
DPM SIMULATION

spouted bed

$$u_{sf} / u_{mf} = 16.0 \leftrightarrow u_{bf} / u_{mf} = 1.2$$



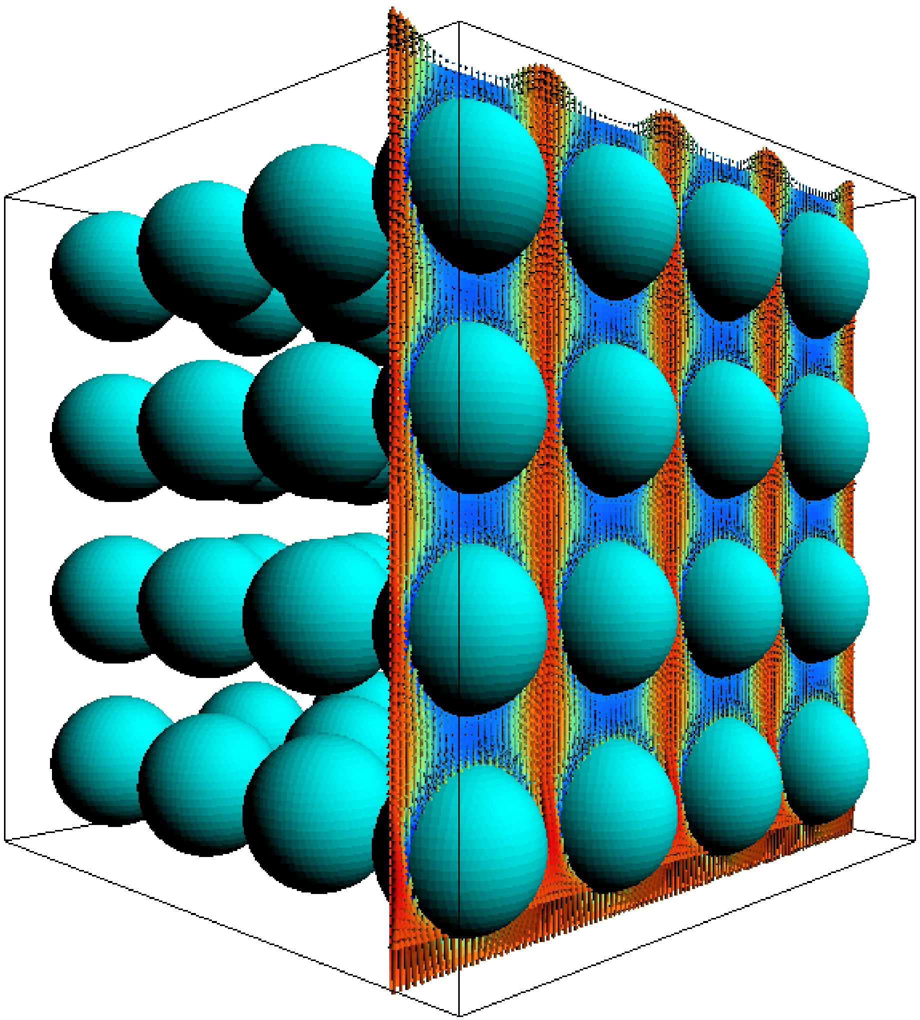
experimental



simulated

DNS (IBM)

flow through cubic array of 64 particles at Re_p=2.0



100^3 Eulerian grid

N=(d_p/h)=20

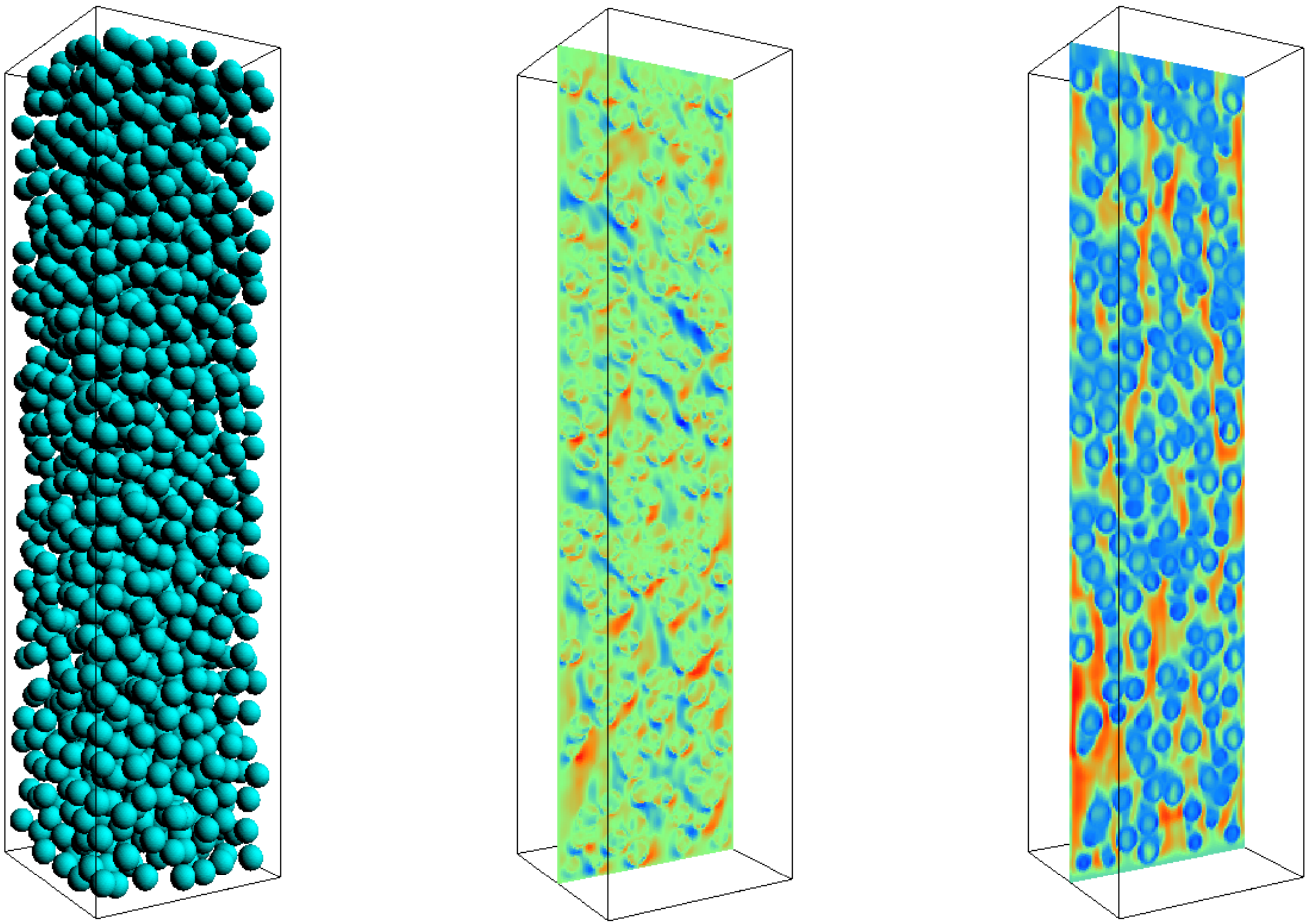
Dimensionless drag

F=10.9 (computed)

F=10.2 (analytical)

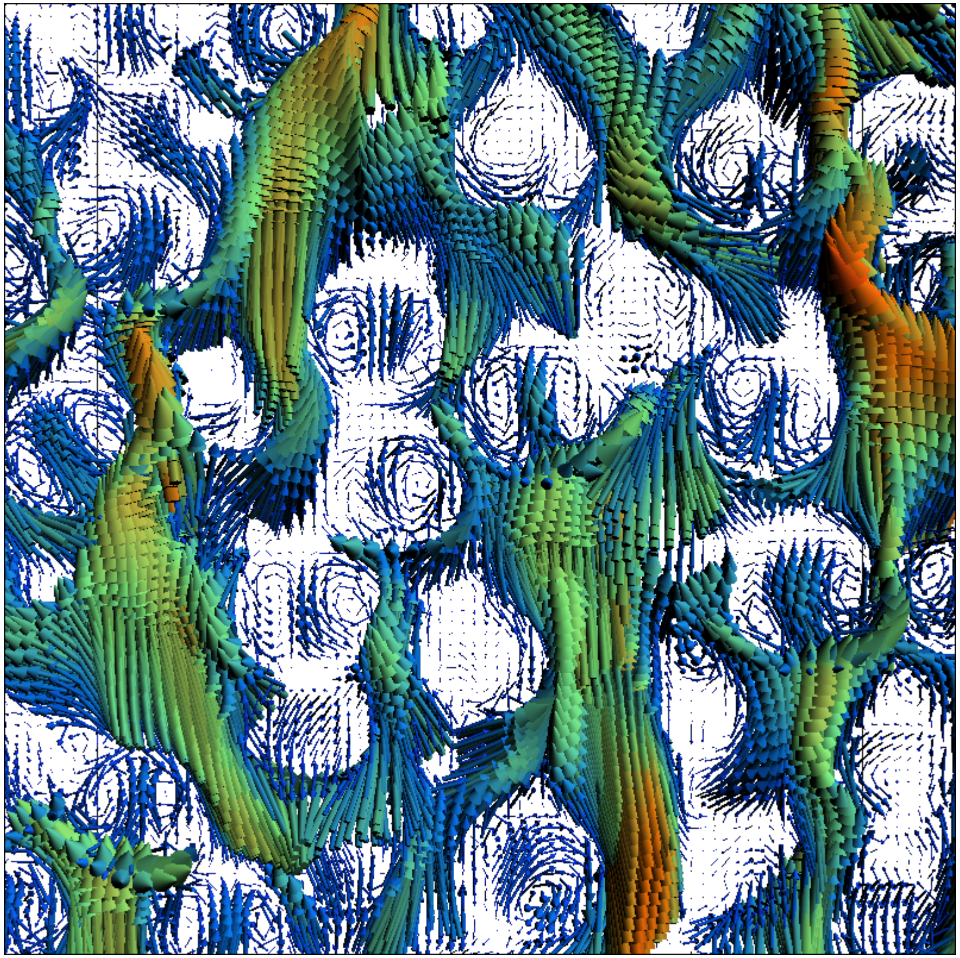
DNS (IBM)

flow through random array of 1326 particles at Re_p=120



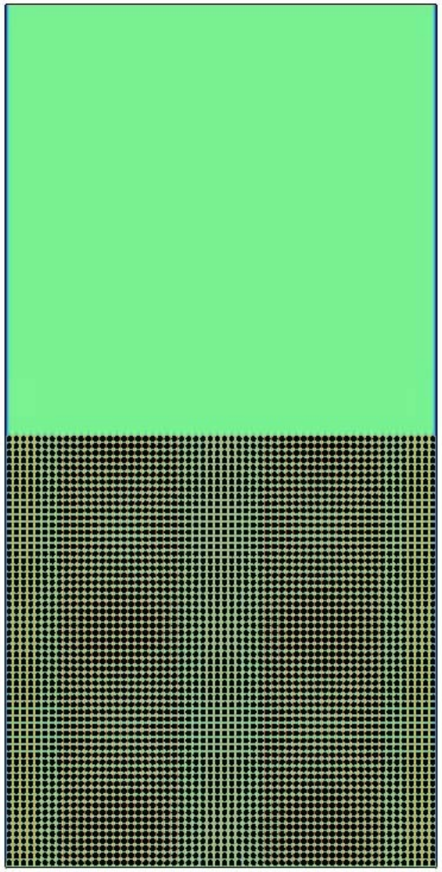
DNS (IBM)

flow through random array of 1326 particles at Re_p=120



DNS (IBM)

fluidization of 3600 discs



KINETIC THEORY BASED MODELS

- BASIC FEATURES

  + statistical mechanical description of particle-particle encounters

- ADVANTAGES

  + based on more fundamental description of particle-particle interaction compared to classical two-fluid model

- DISADVANTAGES

  + incorporation of different particle properties (polydispersity) is quite difficult and leads to (many) additional equations (CPU limitations)

KINETIC THEORY BASED MODELS

- LIMITATIONS AND PRESENT DIFFICULTIES

  + nearly spherical particles

  + not suited for dense gas-particle flows where (quasi-)static particle zones prevail (hoppers, fixed beds and moving beds)

  + incorporation of detailed particle-particle interaction models difficult

  + systems with broad distribution in physical properties (size, density)

  + systems with (rapid) changes in particle size (polymerization)

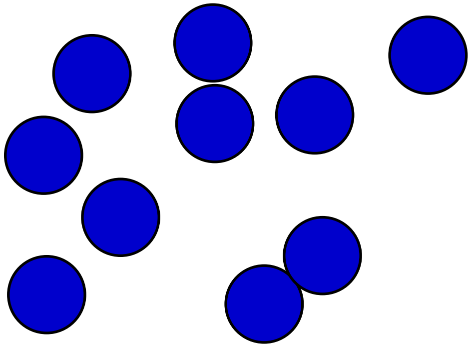
CONTINUUM MODEL BASED ON KINETIC THEORY

- DEFINITION OF PARTICLE VELOCITIES

+ instantaneous particle velocity: $\bar{c}$

+ ensemble averaged particle velocity: $\bar{v}$

+ fluctuating particle velocity: $\bar{C} = \bar{c} - \bar{v}$



- DISTRIBUTION OF FLUCTUATING VELOCITIES (KTG)

$$f = n\left(\frac{m}{2\pi kT}\right)^{3/2} \exp\left(-\frac{mC^2}{2kT}\right)$$

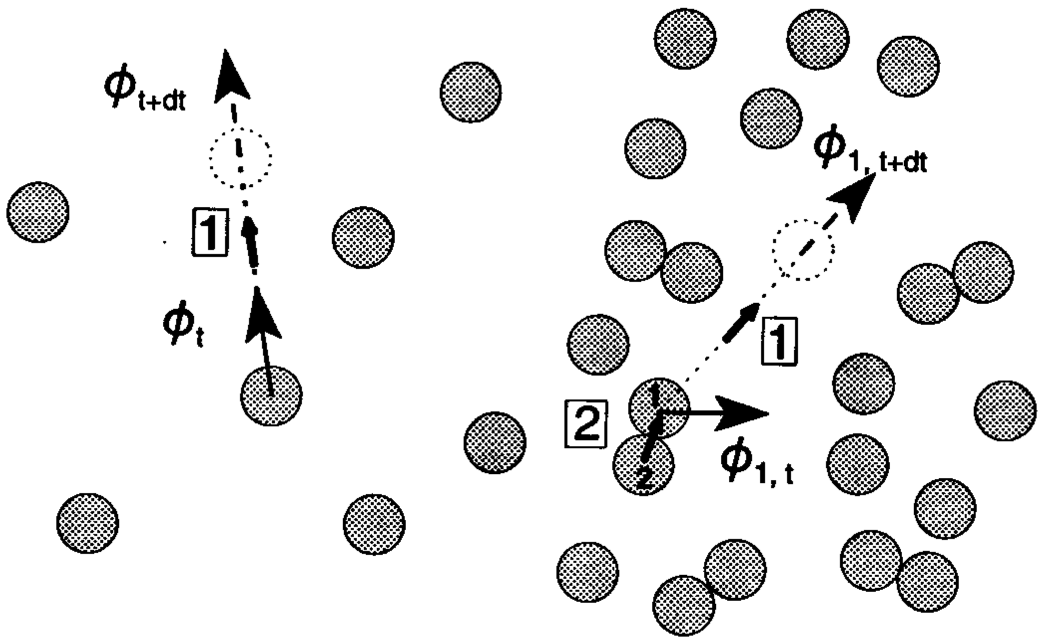
Maxwell's velocity distribution

number density

Boltzmann constant

CONTINUUM MODEL BASED ON KINETIC THEORY

- TRANSPORT MECHANISMS FOR PARTICLE PROPERTY ϕ



CONTINUUM MODEL BASED ON KINETIC THEORY

- BOLTZMANN EQUATION IN TERMS OF $\bar{c}$

$$\frac{\partial f}{\partial t} + (\bar{c} \bullet \frac{\partial f}{\partial \bar{r}}) + (\bar{F} \bullet \frac{\partial f}{\partial \bar{c}}) + f(\frac{\partial}{\partial \bar{c}} \bullet \bar{F}) = (\frac{\partial_e f}{\partial t})$$

- BOLTZMANN EQUATION IN TERMS OF $\bar{C} = \bar{c} - \bar{v}$

$$\frac{Df}{Dt} - (\frac{D\bar{v}}{Dt} \bullet \frac{\partial f}{\partial \bar{\bar{C}}}) + (\bar{C} \bullet \frac{\partial f}{\partial \bar{r}}) - (\bar{C}\, \frac{\partial f}{\partial \bar{\bar{C}}} : \frac{\partial \bar{v}}{\partial \bar{r}}) + (\frac{\partial}{\partial \bar{\bar{C}}} \bullet (f\bar{F})) = (\frac{\partial_e f}{\partial t})$$

- SUBSTANTIAL DERIVATIVE:

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + (\bar{v} \bullet \frac{\partial}{\partial \bar{r}})$$

CONTINUUM MODEL BASED ON KINETIC THEORY

- MAXWELL TRANSPORT EQUATION FOR PROPERTY ϕ

$$\frac{D(n<\phi>)}{Dt} + \left(\frac{\partial}{\partial \bar{r}} \bullet n < \phi \bar{C} >\right) + n < \phi > \left(\frac{\partial}{\partial \bar{r}} \bullet \bar{v}\right) -$$

$$n\left[< \frac{D\phi}{Dt} > + < \bar{C} \bullet \frac{\partial \phi}{\partial \bar{r}} > + < \bar{F} \bullet \frac{\partial \phi}{\partial \bar{\bar{C}}} > - \left(\frac{D\bar{v}}{Dt} \bullet < \frac{\partial \phi}{\partial \bar{\bar{C}}} >\right) -\right.$$

$$\left.\left(\frac{\partial \bar{v}}{\partial \bar{r}} : < \bar{C} \frac{\partial \phi}{\partial \bar{\bar{C}}} >\right)\right] = n\Delta < \phi > = \iiint \phi \left(\frac{\partial_e f}{\partial t}\right) d\bar{C} =$$

- ENSEMBLE AVERAGE OF PROPERTY ϕ

$$< \phi > = \iiint \phi f d\bar{C}$$

$$\boxed{\begin{aligned} &\phi = 1 \\ &\phi = m\bar{C} \\ &\phi = \frac{1}{2} m(\bar{C} \bullet \bar{C}) = \frac{1}{2} mC^2 \end{aligned}}$$

MICRO BALANCE EQUATIONS

- CONTINUITY EQUATIONS

$$\frac{\partial}{\partial t}(\varepsilon_f \rho_f) + (\nabla \cdot \varepsilon_f \rho_f \overline{u}) = 0$$

$$\frac{\partial}{\partial t}(\varepsilon_s \rho_s) + (\nabla \cdot \varepsilon_s \rho_s \overline{v}) = 0$$

- MOMENTUM EQUATIONS

$$\frac{\partial}{\partial t}(\varepsilon_f \rho_f \overline{u}) + (\nabla \cdot \varepsilon_f \rho_f \overline{u}\overline{u}) = -\varepsilon_f \nabla p - (\nabla \cdot \varepsilon_f \tau_f) - \beta(\overline{u} - \overline{v}) + \varepsilon_f \rho_f \overline{g}$$

$$\frac{\partial}{\partial t}(\varepsilon_s \rho_s \overline{v}) + (\nabla \cdot \varepsilon_s \rho_s \overline{v}\overline{v}) = -\varepsilon_s \nabla p - (\nabla \cdot \varepsilon_s \tau_s) - \nabla p_s + \beta(\overline{u} - \overline{v}) + \varepsilon_s \rho_s \overline{g}$$

MICRO BALANCE EQUATIONS

- GRANULAR TEMPERATURE EQUATION

$$\frac{3}{2}\left[\frac{\partial}{\partial t}(\varepsilon_s \rho_s \Theta) + (\nabla \cdot \varepsilon_s \rho_s \Theta \bar{v})\right] = -(p_s I + \varepsilon_s \tau_s) : (\nabla \bar{v}) + (\nabla \cdot \varepsilon_s \kappa_s \nabla \Theta) + \beta[\overline{\bar{c}_f \cdot \bar{c}_s} - 3\Theta] - \gamma$$

- ADDITIONAL EQUATIONS AND CLOSURES

for dense flows this term can safely be neglected

+ phase densities
+ phase stress tensors and phase viscosities
+ pseudo Fourier energy flux and solids pseudo conductivity
+ solids pressure
+ interphase momentum exchange coefficient
+ covariance between fluid and solid fluctuating velocities

CLOSURE OF MICRO BALANCE EQUATIONS

interphase momentum transfer coefficient

- Ergun equation (ε_f<0.8):

$$\beta = 150\frac{(1-\varepsilon_f)^2}{\varepsilon_f}\frac{\mu_f}{d_p^2} + 1.75(1-\varepsilon_f)\frac{\rho_f}{d_p}\left|\bar{u}-\bar{v}\right|$$

- Wen and Yu equation (ε_f>0.8):

$$\beta = \frac{3}{4}C_d\frac{\varepsilon_f\varepsilon_s}{d_p}\rho_f\left|\bar{u}-\bar{v}\right|\varepsilon_f^{-2.65}$$

exponent depends on particle Reynolds number Re_p

- Drag coefficient:

$$\mathrm{Re}_p = \frac{\varepsilon_f\rho_f\left|\bar{u}-\bar{v}\right|d_p}{\mu_f}$$

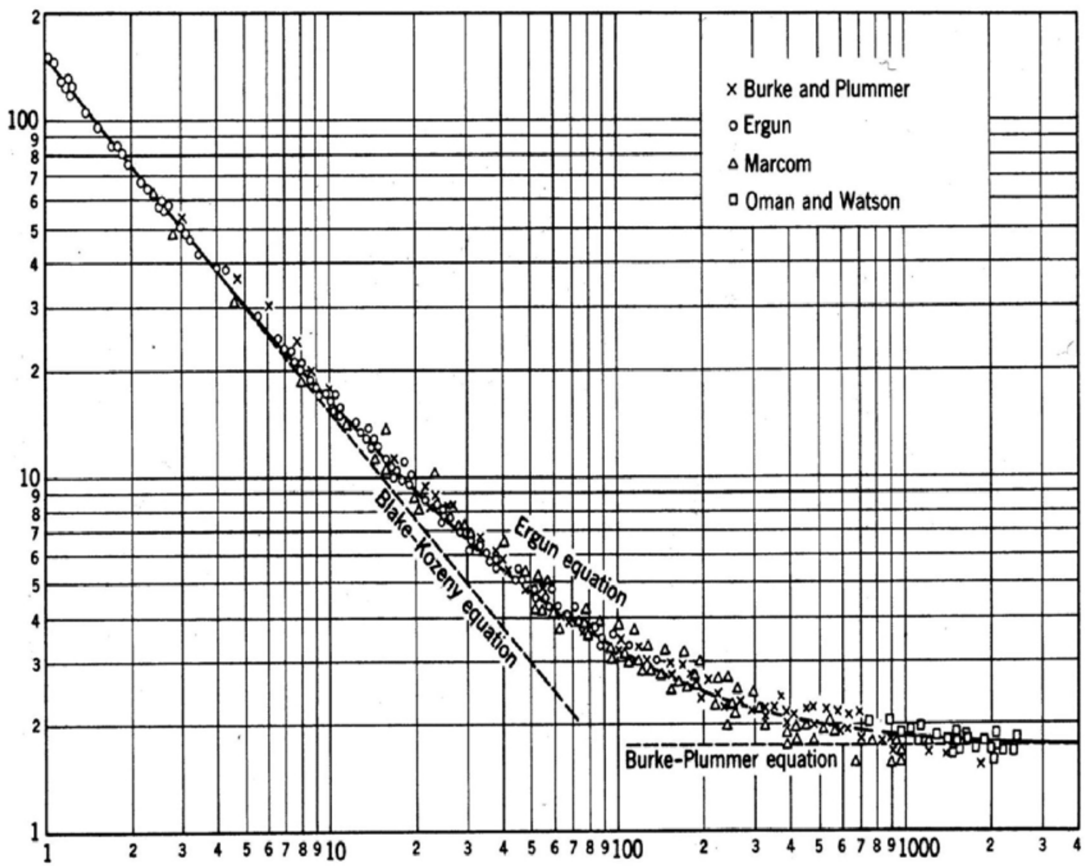
$$C_d = \frac{24}{\mathrm{Re}_p}[1+0.15(\mathrm{Re}_p)^{0.687}]$$

$$C_d = 0.44$$

Re_p<1000 **Re_p>1000**

DRAG CLOSURE

Ergun equation



$F * \left(\frac{18\epsilon}{Re}\right)$

$Re/(1-\epsilon)$

CONTINUUM MODEL BASED ON KINETIC THEORY

- SUMMARIZING THE KEY FEATURES OF KTGF

+ particles interact through binary nonideal collisions (no friction)

+ non-ideal particle-wall collisions are accounted for

+ departure from Maxwellian (velocity) distribution function is small

+ one additional equation (“granular temperature equation”)

+ closures for solids viscosity, pressure and pseudo conductivity

+ random granular motion and no collective granular motion

NUMERICAL SOLUTION METHOD

- KEY FEATURES

+ explicit treatment of convection and diffusion terms

$$\left[\frac{|u_x|}{\Delta x}+\frac{|u_y|}{\Delta y}+\frac{|u_z|}{\Delta z}\right]\Delta t<1 \qquad \nu_f \Delta t < \frac{1}{2}[\frac{1}{\frac{1}{(\Delta x)^2}+\frac{1}{(\Delta y)^2}+\frac{1}{(\Delta z)^2}}]$$

stability conditions

$$\left[\frac{|v_x|}{\Delta x}+\frac{|v_y|}{\Delta y}+\frac{|v_z|}{\Delta z}\right]\Delta t<1 \qquad \nu_s \Delta t < \frac{1}{2}[\frac{1}{\frac{1}{(\Delta x)^2}+\frac{1}{(\Delta y)^2}+\frac{1}{(\Delta z)^2}}]$$

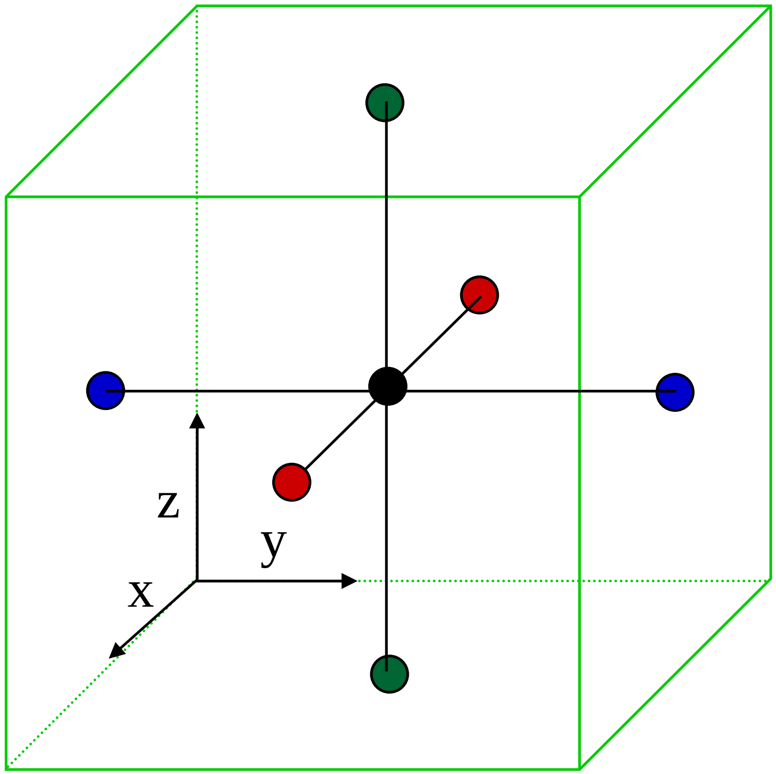
+ implicit treatment of porosity pressure in momentum equations

+ staggered computational mesh

+ high order schemes for convection for mass <u>and</u> momentum

NUMERICAL SOLUTION METHOD

- DEFINITION OF EULERIAN VARIABLES



- scalar variables
- x-velocity component
- y-velocity component
- z-velocity component

NUMERICAL SOLUTION METHOD

- OVERALL COMPUTATIONAL STRATEGY PER CYCLE

compute convection and diffusion terms for g+s momentum equations

⇓

estimate g+s velocity distributions using old porosity + pressure fields

⇓

solve porosity and pressure Poisson equations using ICCG

⇓

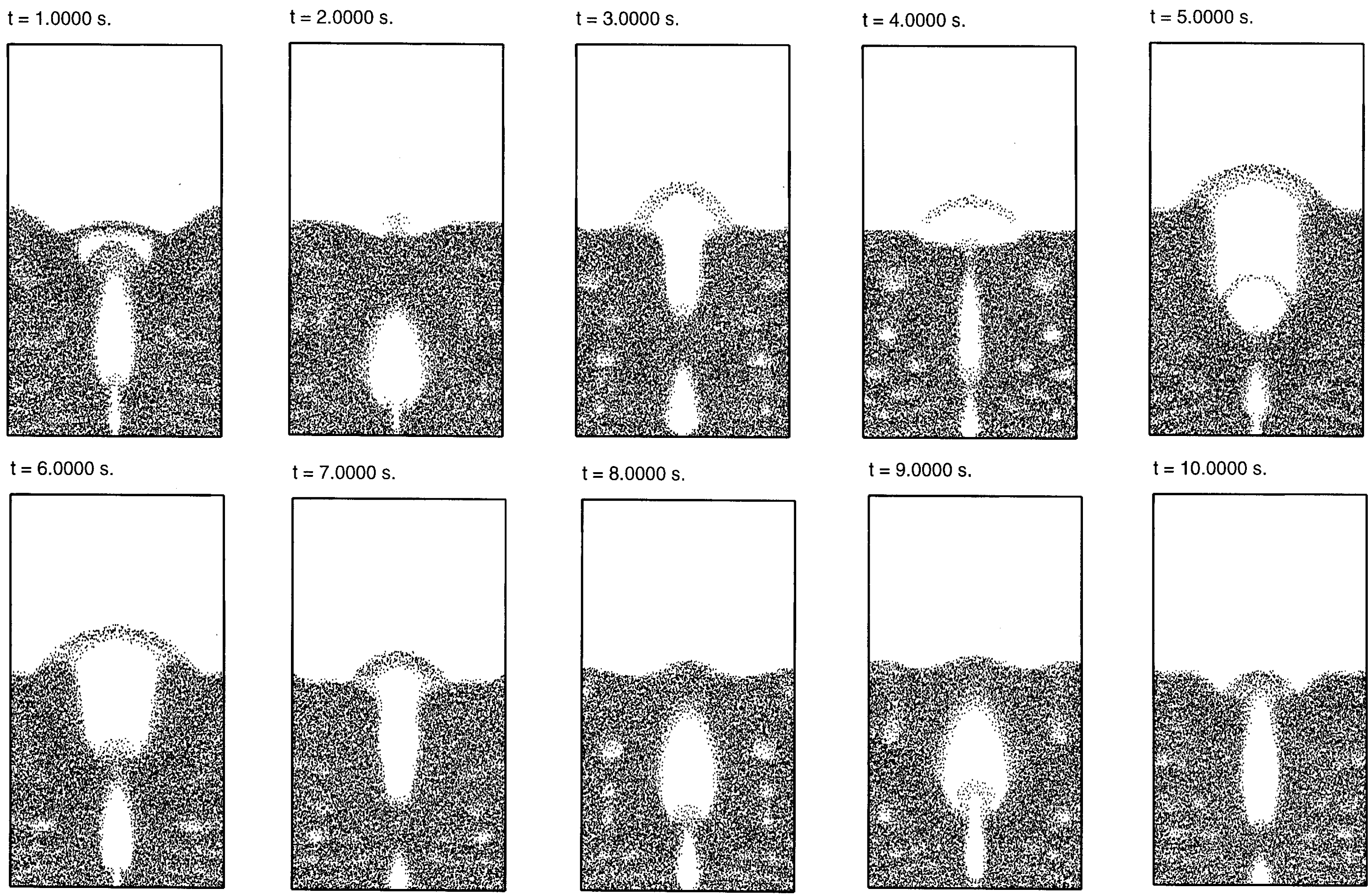
compute g+s velocity distributions with new porosity + pressure fields

⇓

solve granular temperature equation

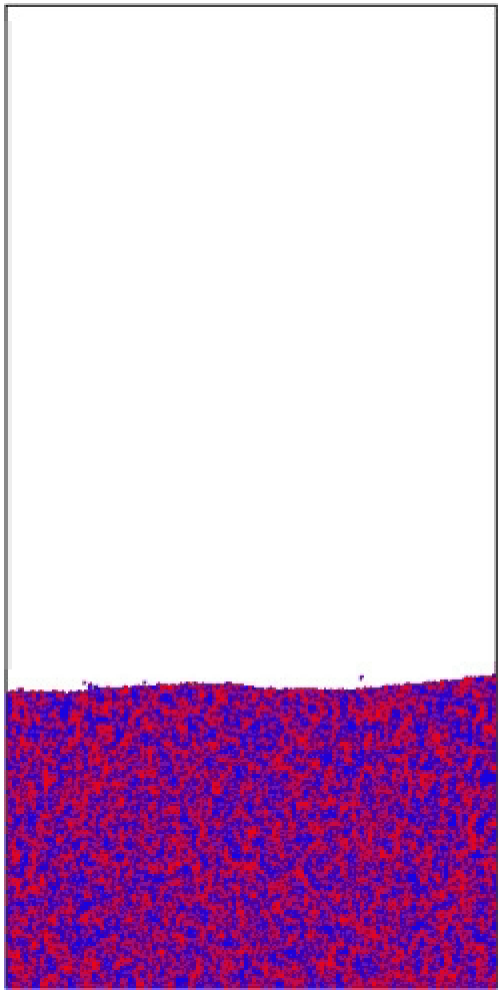
RESULTS OF KTGF MODEL

bubble formation at a jet using 3D model

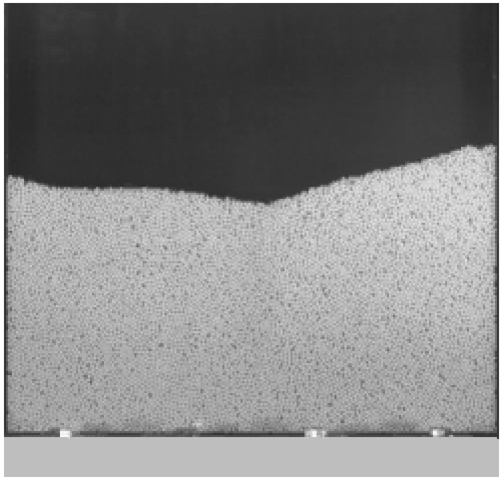


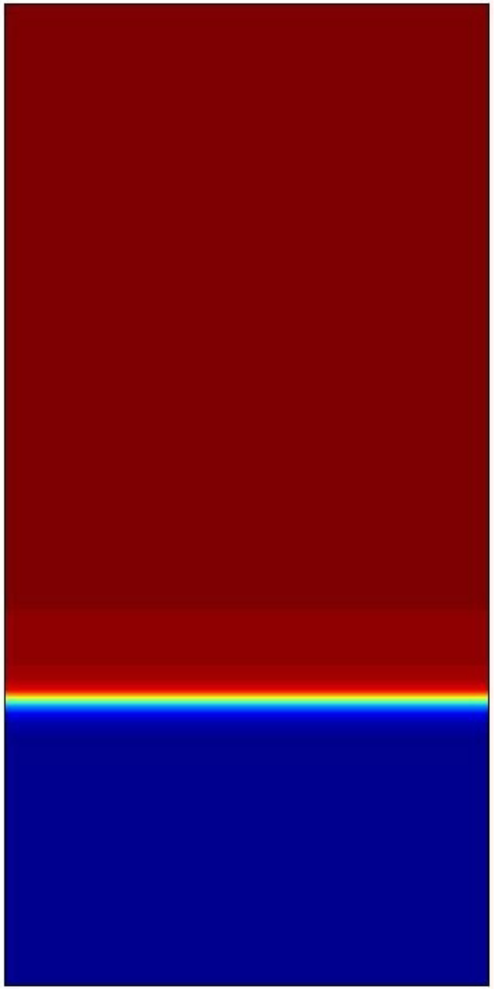
RESULTS OF KTGF MODEL: MONODISPERSE SYSTEMS

bubble formation: 30 cm bed



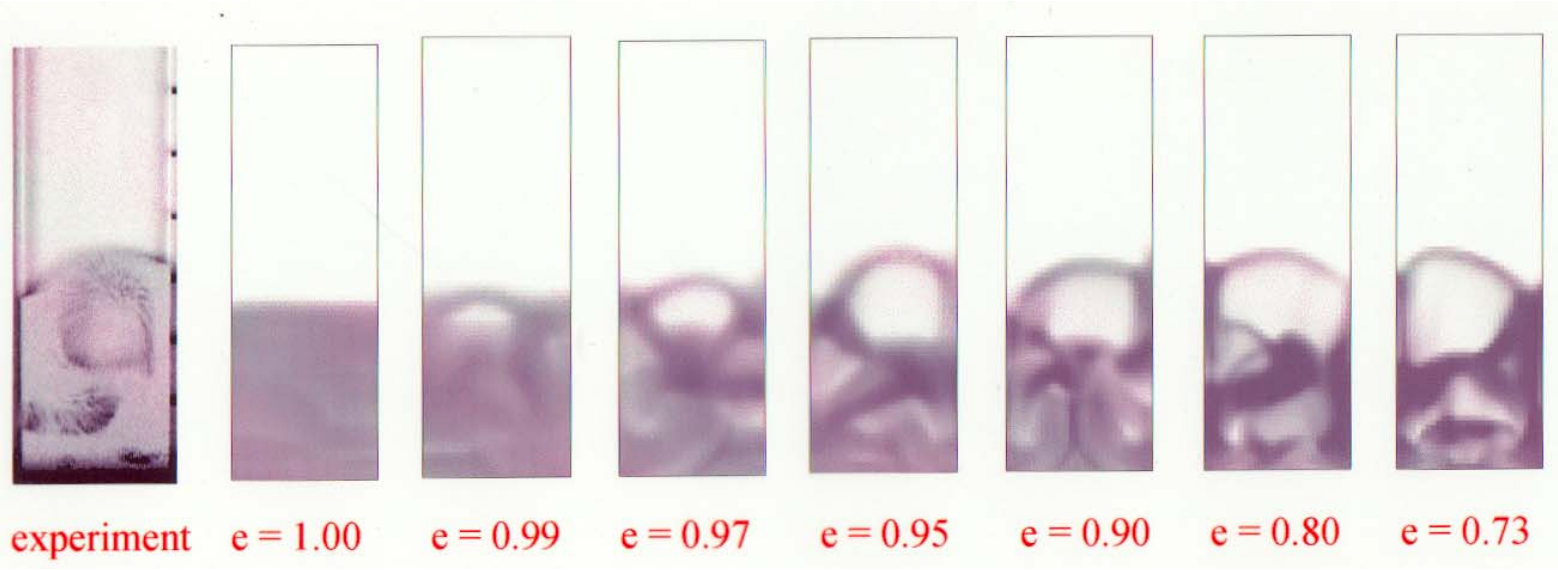
W=0.30 m
d_p=2.5 mm
ρ_s=2526 kg/m^3
U_b=1.20 m/s
U_j=20.0 m/s
N_p=60000





RESULTS OF KTGF MODEL

effect of restitution coefficient on bed dynamics



RESULTS OF KTGF MODEL

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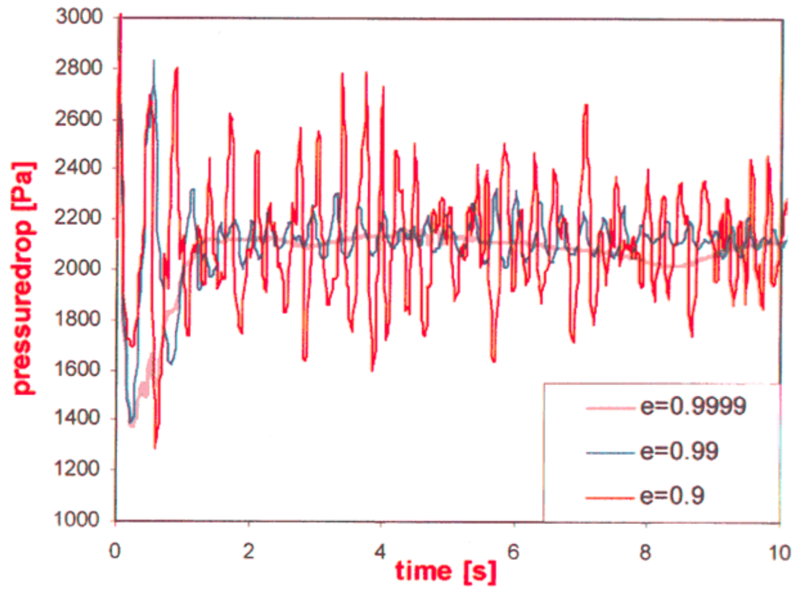
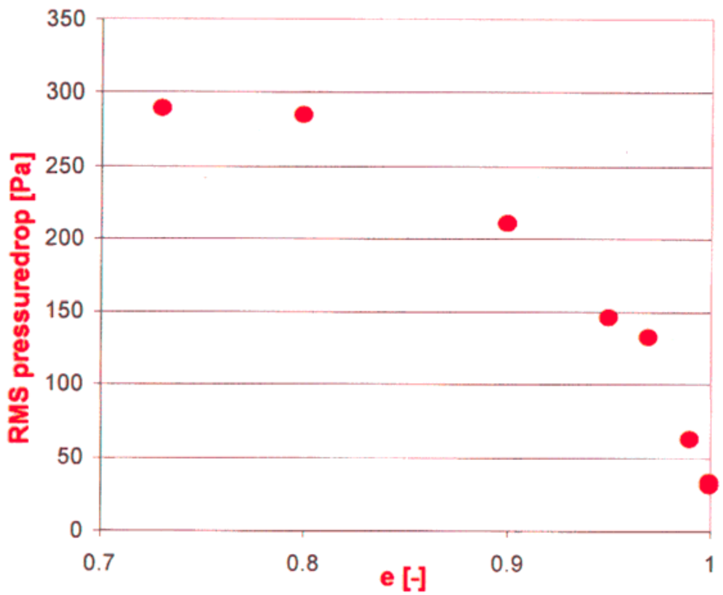
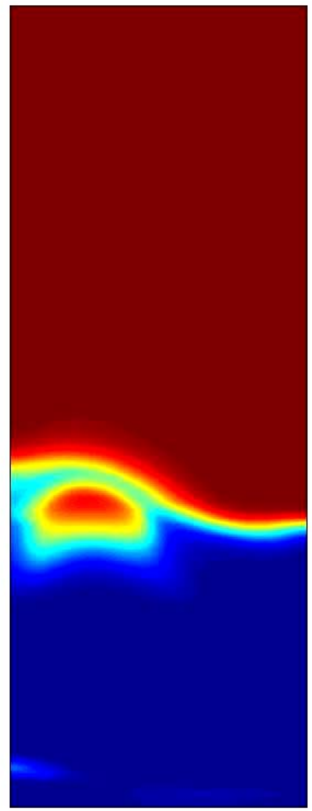
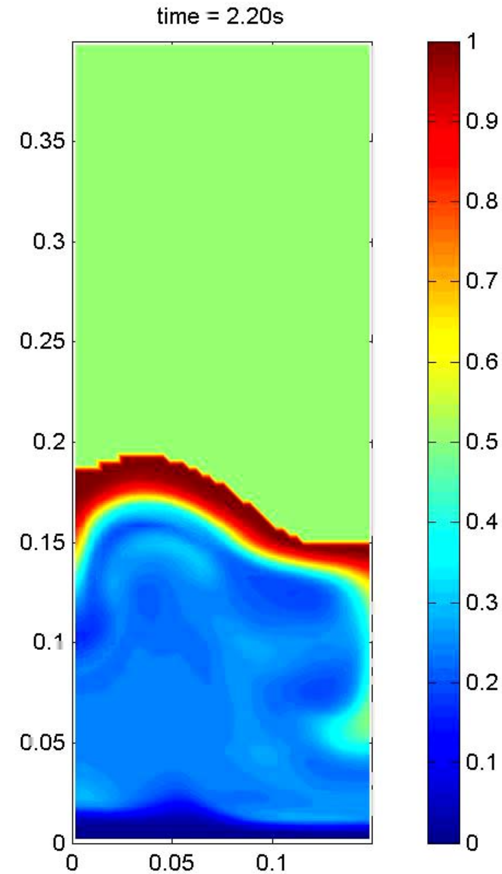




RESULTS OF KTGF MODEL: BIDISPERSE SYSTEMS

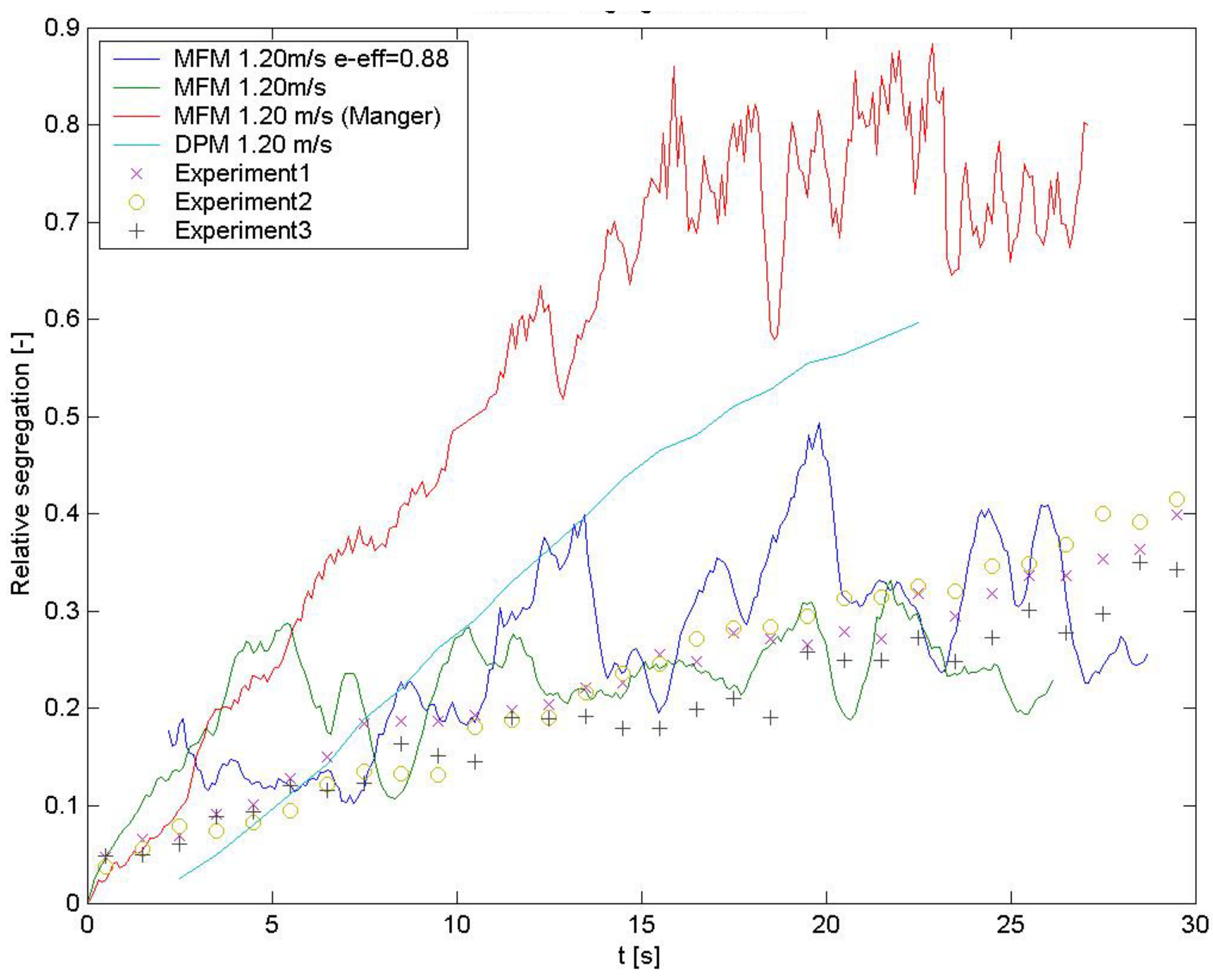
segregation rate in bidisperse systems





RESULTS OF KTGF MODEL: BIDISPERSE SYSTEMS

segregation rate in bidisperse systems



RESULTS OF KTGF MODEL

effect of lateral segregation on riser reactor performance

- RISER FLOW

+ particle diameter (FCC)	40 μm
+ riser diameter	0.3 m
+ superficial gas velocity	6.3 m/s
+ solids mass flux	390 kg/(m^2.s)

- FEATURES

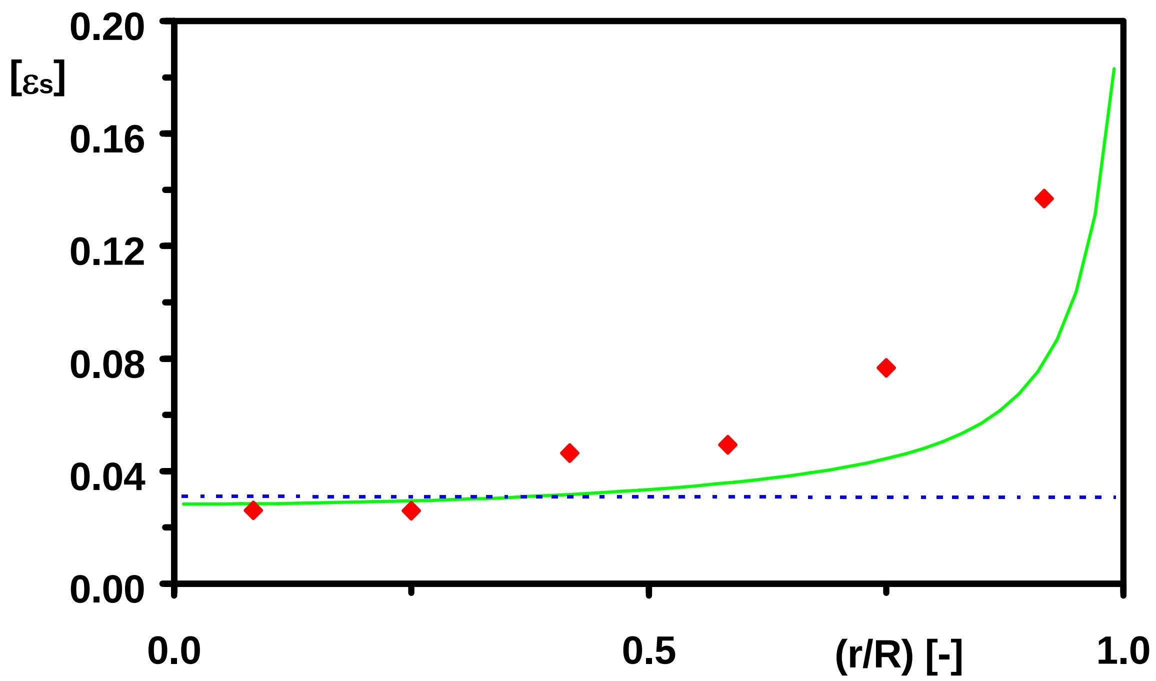
+ two-fluid model incorporating kinetic theory of granular flow
+ turbulence model: Prandtl mixing length model
+ axi-symmetrical flow

RESULTS OF KTGF MODEL

effect of lateral segregation on riser reactor performance

- RISER FLOW

RADIAL PROFILE OF SOLIDS VOLUME FRACTION ε_s

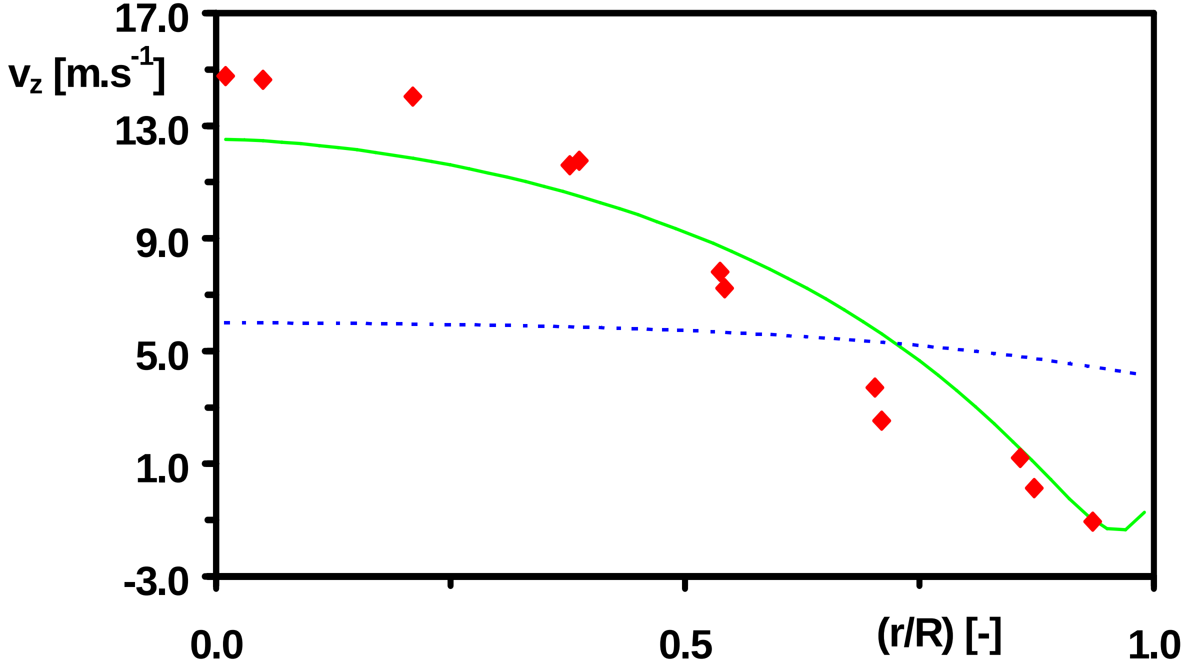


RESULTS OF KTGF MODEL

effect of lateral segregation on riser reactor performance

- RISER FLOW

RADIAL PROFILE OF AXIAL SOLIDS VELOCITY V_z



RESULTS OF KTGF MODEL

effect of lateral segregation on riser reactor performance

- REACTION SCHEME:

$$A + [*] \xrightarrow{k_1} B + [*] \xrightarrow{k_2} C + [*]$$

$$[*] \xrightarrow{k_3} [-]$$

- KINETICS:

$$r_A = -\varepsilon_s [*] \rho_f k_1 x_A$$

$$r_B = +\varepsilon_s [*] \rho_f (k_1 x_A - k_2 x_B)$$

$$r_C = +\varepsilon_s [*] \rho_f k_2 x_B$$

$$r_* = -\varepsilon_s [*] \rho_s k_3$$

$$k_1 = 25\ s^{-1}$$

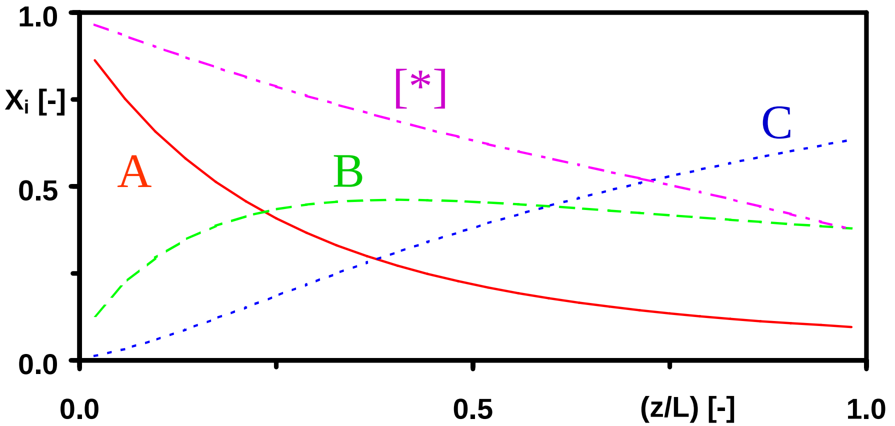
$$k_2 = 15\ s^{-1}$$

$$k_3 = 0.2\ s^{-1}$$

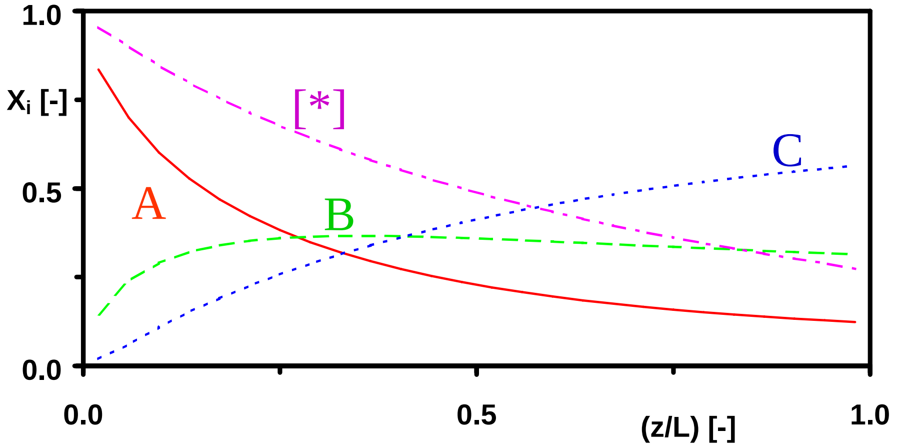
RESULTS OF KTGF MODEL

effect of lateral segregation on riser reactor performance

- AXIAL PROFILE OF FLOW-AVERAGED FRACTIONS IN RISER



IDEAL



NON-IDEAL

CONCLUSIONS

- BUBBLING BED

  + significant effect of e on bubble dynamics

  + dissipation level to low (friction is not included in KTGF)

- CFB RISER

  + radial segregation in dense riser flow can be predicted

  + significant effect of radial segregation on riser reactor performance