Computational Studies on Gas-Solid Fluidization of Geldart A Particles Using Eulerian-Eulerian Two-Fluid Model

THESIS

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by

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DEDICATED

TO

My Family and Friends

BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE

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CERTIFICATE

This is to certify that the thesis entitled **"Computational fluid dynamic (CFD) study on gas-solid fluidization of Geldart A particles"** submitted by **Priya Christina Sande,** ID No. **2007PHXF014P** for the award of PhD Degree of the Institute, embodies the original work done by her under my supervision.

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ABSTRACT

Today computational fluid dynamics (CFD) is a partner with pure theory and pure experiment in the analysis and solution of fluid dynamic problems. In this work CFD has been used as a research tool to gain insight into the fluidization of Geldart A particles. Qualitative and quantitative investigation of homogeneous expansion and transition to bubbling was carried out. The two-phase flow is inherently complex and displays characteristic heterogeneity over different length and time scales which is ideal to be studied by CFD which has the unique feature of giving a visual description of the flow. The homogeneous expansion occurs only for Geldart A particles in the interval between minimum fluidization and free bubbling. The bed is believed to expand in a bubble-free manner; hence the name homogeneous expansion is given. The breakdown of this expansion and onset of bubbles has significance for a reactor and marks the transition to the bubbling regime. The standard Two-Fluid Model (TFM) which follows the *Eulerian-Eulerian* approach was used in conjunction with selected closures from literature without modifications. The TFM was implemented in the FLUENT 6.3.26 CFD solver using finite volume method. PC-SIMPLE algorithm and segregated solver was employed. The investigations are reported in three parts (i) detailed study on mesh size effect (ii) detailed fine mesh study (iii) Reacting bed study.

From the mesh size effect study we found that with mesh refining, minimum bubbling velocity dropped exponentially and approached its experimental value. For capturing homogeneous expansion there was no improvement at all on reducing mesh size up to 1mm × 1mm from the commonly used literature value of 4mm × 4mm. Review of over 150 simulations across all the mesh sizes studied, revealed the presence of persisting dilute regions, instead of bubbles, which get triggered around experimental minimum bubbling velocity of approximately 8mm/s. Theses dilute regions were proposed as a marker which signals the onset of bubbling regime for the coarse mesh simulations. The effect of using frictional stress model in the simulations was qualitatively assessed. Also the effect of changing wall boundary condition for both gas and particle phase was investigated. Omitting frictional stress or changing no-slip to free-slip boundary condition for gas phase resulted in delaying minimum bubbling velocity. The effect of commonly used drag laws was also studied and it was found that the Gidaspow and Syamlal O'Brien drag laws manifested the dilute region markers at 8mm/s while for Wen Yu drag law this value was 10mm/s.

From the fine mesh (0.4mm × 0.4mm) simulations of lab-scale dimensions the hydrodynamics of homogeneous regime and transition to bubbling were studied in detail. The effect of particle density was investigated in detail. The fine mesh simulations were analyzed for: (i) insights into bed transition from homogeneous to bubbling regime (ii) effect of inter-particle forces (IPFs) and (iii) Geldart group A to B transition. Simulations reveal that transition to bubbling occurs over a velocity *range* rather than at a discrete velocity. Based on observations of over 25 fine mesh simulations the existence of a *transition regime* was proposed between the well known homogeneous and bubbling regime. For the first time we attempted to *quantify* the overall effect of IPFs from CFD simulations. The proposed IPF index dropped exponentially and becomes negligible as bubbling ensued. TFM simulation results were found comparable to *Eulerian-Lagrangian* simulations and also experimental data. Fine mesh simulations revealed two or three void structures not previously resolved, but more importantly much finer variations in the dilute regions. Fine mesh simulations could predict the bubbling transition, though it did

not adequately capture the Richardson-and Zaki type experimentally observed homogeneous expansion. This was shown to be due to the over prediction of the component of voidage due to frictional viscosity. Without frictional stress component the Richardson-and Zaki type expansion was clearly observed, showing that the commonly used frictional stress model over estimates bed voidage in homogeneous expansion regime. The Richardson-and Zaki parameter (*n*) was obtained and analyzed for the homogeneous expansion regime and transition regime. The *n* values decreased with terminal Reynolds number as observed in literature for liquid systems. However, the *n* values themselves were higher than those reported for liquid systems. TFM simulations show that the transition from Geldart group A to B occurs more gradually than is indicated by the Geldart classification chart. The area over which this transition occurs was demarcated on the Geldart chart.

The oxychlorination of ethylene reaction was simulated in three modes: (i) fixed bed (ii) Bubbling bed; and (iii) Homogeneous bed. Hydrodynamics was modeled using TFM, and reaction kinetics obtained from literature was incorporated via a user defined function (UDF). The simulated reaction rates for the fixed bed were validated with experimental values from literature. The simulated conversion was highest for the homogeneous bed, second highest for the bubbling and least for the fixed bed. This was mainly because conversion is directly proportionate to gas residence time, which was highest for homogeneous bed and least for fixed bed. Fixed bed had the highest average bed reaction rates when compared to homogeneous and bubbling bed. This was because reaction rate was directly proportionate to solid packing, which was highest in fixed bed. Further, the average reaction rates for the homogeneous bed were only marginally lower than that of the bubbling bed. Hence the homogeneous bed combined optimum solid packing (between that of fixed and bubbling bed) with long gas residence times, to give highest conversion at reaction rates comparable to bubbling bed.

Keywords: *Eulerian-Eulerian*; *CFD simulations; Fluidization; Geldart A particles; Two-fluid model; Homogeneous expansion; Fine mesh; minimum bubbling transition, Gidaspow drag law; Syamlal O'Brien Frictional stress law, Richardson-Zaki expansion, Inter-particle forces, Oxychlorination of ethylene, fixed bed, bubbling bed, homogeneous bed.*

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NOMENCLATURE

$\overline{A}$	Material constant required to calculate frictional pressure, typical value 10^{25}
D_a, m_a, V_a	Displacement (m), mass (kg) and volume (m^3) of particle '*a*'
d_p	Particle diameter (μm)
e_s	Restitution coefficient for particle collision (-)
F_{45}	Mass fraction of particles with $d_p < 45$ μm
$\overline{Fr}, \overline{p}, \overline{n}$	Empirical material constants required to calculate pressure (-)
$F_{c,a}, F_{vdw,a}, F_{drag,a_a}$	Contact force, van der Waals force, drag force for particle '*a*'
$\overrightarrow{g}$	Acceleration due to gravity (m/s)
$g_{o,s}$	Radial distribution function (-)
H	Experimentally measured height of bed (m)
H_{ab}	Hamaker constant for interparticle forece between particles '*a*' and '*b*'
$\overline{\overline{I}}$	Unit stress tensor (-)
K_{gs}	Momentum exchange coefficient between gas and solid phase (-)
$\dot{m}_{sg}$	Mass transfer rate from solid to gas phase (kg/s)
$\dot{m}_{gs}$	Mass transfer rate from gas to solid phase (kg/s)
n	Richardson-Zaki parameter (-)
p	Gas pressure (Pa)
p_s	Solids pressure or solid particles bed pressure (Pa)
p_f	Solids pressure due to friction (Pa)
Re_t	Terminal settling Reynolds number ($d_p u_t \rho_g / \mu_g$)
S, v_p, u_g	Intersurface particle distance (m), particle velocity (m/s), local gas velocity (m/s)
$u_{mb,e}$	Experimental minimum bubbling velocity for simulated system (8mm/s)
U_{mb}	Minimum bubbling velocity obtained by observation of first bubble from fine mesh simulations (mm/s)
$U_{mb,\ mesh\text{-}size}$	Minimum bubbling velocity (mm/s) obtained by observation of first bubble (mm/s) simulated at given coarse mesh size
u	Superficial gas inlet velocity (m/s)
u_t	Particle terminal fall velocity (m/s)
u'_{mb}	Minimum bubbling velocity obtained by observation of dilute regions from fine mesh simulations (mm/s)
u'_b	Inlet gas velocity for first appearance of clearly defined multiple bubbles in fine mesh simulations (mm/s)
v_s'	Average particle velocity fluctuation (-)
$\overrightarrow{v_s}$	Velocity vector for solid phase (m/s)
$\overrightarrow{v_{gs}}$	Interphase velocity vector $If\ \dot{m}_{gs} > 0, \overrightarrow{v_{gs}} = \overrightarrow{v_g}\ \ else\ if\ \dot{m}_{gs} < 0, \overrightarrow{v_{gs}} = \overrightarrow{v_s}$
$\overrightarrow{v_{sg}}$	Interphase velocity vector $If\ \dot{m}_{sg} > 0, \overrightarrow{v_{sg}} = \overrightarrow{v_s}\ \ else\ if\ \dot{m}_{sg} < 0, \overrightarrow{v_{sg}} = \overrightarrow{v_g}$
$\nabla \overrightarrow{v_s}$	Divergence of solid velocity vector (-)
$\nabla \overrightarrow{v_s}^T$	Transpose of divergence of solid velocity vector

Greek Symbols

ε_s	Solid volume fraction in bed/cell (-)
$\varepsilon, \varepsilon_g$	Gas volume fraction in bed/cell (-)
ε_s^{max}	Maximum bed solid volume fraction or solid packing for packed bed state (-)
ε_s^{min},	Minimum bed solid volume fraction for frictional stress consideration (-)
ρ_{rg}	Reference density or volume average density of gas phase (kg/m^3)
ρ_g	Density of gas phase (kg/m^3)
ρ_s	Density of solid phase (kg/m^3)
ρ_p	Density of particles (kg/m^3)
ϕ	Angle of internal friction (^{o})
Θ	Granular temperature (m^2/s^2)
μ_s	Shear viscosity of solid particles (Pa s)
λ_s	Bulk viscosity of solid particles (Pa s)

Subscripts

g	gas phase
p	particle phase
mf	minimum fluidization
mb	minimum bubbling
sim	Simulated
exp	experimental
extrap	extrapolated

Abbreviations

BC	Boundary condition
CGR	Chemical Growth Rate
DEM	Discrete Element Method
DPM	Discrete particle Model
EDC	Ethylene dichloride
FS	Frictional Stress
IPFs	Interparticle forces
QUICK	Quadratic Upstream Interpolation for Convective Kinematics
R-Z	Richard and Zaki
SC	Specularity Coefficient
SIMPLE	Semi-Implicit Method for Pressure-Linked Equations
TFM	Two Fluid Model
UDF	User Defined Function
VOF	Volume Of Fluid (model)