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Mathematical model for Hydrodynamics and heat transfer

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Abstract:
A circulating two-phase Taylor flow in a microchannel was considered to be more efficient for overall heat transfer in a heat pipe compared to the pulsating (oscillating) heat pipe. A mathematical model describing the main parameters of a two-phase flow is constructed. The experimental study of hydrodynamics and heat transfer of a circulating two-phase (liquid–vapor) Taylor flow in a glass microchannel was performed. The experimental studies confirmed a microchannel heat pipe operability with a two-phase flow in a circulating mode. Various combinations of heater and cooler disposition have been examined. Minimal heating power to establish Taylor flow was found experimentally for each combination. The numerical procedure is applied in layers of infinitesimal height, in order to be possible to solve the energy, the momentum and the continuity equations, and an irregular mesh was used. The bubbling portion of the bed and the splash zone are composed, each one, by a single layer; this approach is a function of the hydrodynamic model upon which the heat transfer model is based. For the core-annulus zone, two columns of infinitesimal layers were used. In fact several meshes are used, concerning fluid-dynamic properties, heat transfer properties and geometrical features.

Key words: Circulating Fluidised Bed Boilers; Heat Transfer; Numerical Modelling, Biomass.

I. Introduction

Circulating fluidized beds involving combustion or exothermic reaction commonly require heat transfer to the bed walls. The heat transfer helps to control the bed temperature and serves as a primary means to generate steam or hot water from the bed. Circulating beds are characterized by a substantial variation in average cross-sectional solids density from the distributor to the outlet; there may be corresponding variations in local bed-to-wall heat transfer with bed height. It is important to design the bed for the proper rate of heat transfer. Overestimating the rate of heat transfer to the walls results in the need for additional heat transfer surface or operation at elevated bed density, which presents a penalty in fan operating power [1]. There is no guarantee that heat transfer results obtained in a laboratory bed or pilot plant are directly transferable to a much larger commercial design. 1 General observations Heat transfer results are reported in terms of the heat transfer coefficient, h, which relates the rate of heat transfer from the bed to the surface to the overall temperature difference and the surface area:

$$q = hA(T_{bed} - T_{wall}) \quad 1)$$

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Although the gas or particles near the wall may undergo a temperature change it is more convenient to write h in terms of the difference between the mean bed temperature at the cross-section in question and the wall temperature. q and h may be defined for a small local area or may be quantities averaged over a large area of the surface. Observations of heat transfer in both small-scale laboratory columns and larger commercial beds indicate that h increases with the cross-sectional average solids density. h also increases with elevated temperatures. When the superficial gas velocity is varied, if the solids recycle rate is also adjusted to keep the cross-section average solids density constant, h varies little, if at all. In some instances, h is found to increase when the mean particle diameter is decreased [2]. The vertical length of the active heat transfer surface influences h: longer surfaces result in lower values of h as well as a decreased influence of particle size. Finally, h tends to increase with bed diameter at a fixed cross-sectional-averaged particle concentration.

Preliminary evidence indicates that h is also a function of surface roughness; even small amplitude roughness may lead to noticeable changes in h. Although the interest in circulating fluidized beds has increased substantially over the past decade, our understanding of their hydrodynamics and heat transfer is still far short of the state of knowledge for bubbling fluidized beds. At present, there is not a definitive set of experimental data or predictive models that allow designers to predict confidently the heat transfer rate for a new circulating bed design. There is a dearth of information available for large commercial units. The goal of the present chapter is to develop a physical understanding of the heat transfer process in circulating beds. We will show that heat transfer is intimately tied to hydrodynamics, especially to particle and gas behavior close to the heat transfer surface [3]. The hydrodynamic behavior near the wall, as best we understand it, will help us gain an understanding of general trends in observed heat transfer behavior and lead to simple predictive models.

A number of different models have been proposed. Each requires several key parameters which are known, at best, approximately. Given the uncertainty in the required parameters, models that are unnecessarily detailed or complex are unwarranted and do not lead to better predictive capability. Emphasis is given to models that are straightforward and incorporate the relevant physics. The great majority of available heat transfer data were obtained from small laboratory-scale beds. These are reviewed in light of the physical models with an eye toward validity, general correlation, and extrapolation of the results to commercial-scale systems. Trends of the data, in many cases, can be explained by proper understanding of the physical process.

Hydrodynamics Our primary focus will be on heat transfer between a circulating bed and the bed walls. The heat transfer process is controlled by the hydrodynamics of the solid and gas mixture in the vicinity of the wall. Although the wall hydrodynamics is important to heat transfer, relevant information has only recently come to light. As described in previous chapters, the overall structure of a circulating or fast bed includes a core with clusters of particles and individual particles moving upward in the gas stream [4]. The particles actively circulate in the core where the temperature is near uniform. In an annular region near the walls where the gas

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velocity is reduced, the particles tend to fall downward. The width of this zone, whose boundary is commonly defined as the point where the net solid flux (upward minus downward) is zero, tends to be a modest portion of the bed diameter.

Clusters or individual particles at the mean bed temperature enter the annular region from the core. There will be a lateral temperature gradient near a cooled wall. The radial deposition of solids from the core to the wall has been likened to a radial diffusion process. Argued that in the upper dilute region of the bed, the radial flux is due primarily to radial motion of dilute collections of particles rather than radial motion of concentrated clusters. (The particles may form more concentrated clusters or strands within the annular region or at the wall inhibiting their motion by diffusion back into the core.) In the lower portion of the bed, particle motion to the wall may be largely due to particles ejected from the dense region near the base of the bed with a radial component of velocity. The downflowing layer near the wall exhibits considerable short-time excursions in local concentration and layer thickness as clusters appear and are replaced by dilute gas-solids mixture.

II. Modeling Variants

With this in mind, an exercise was undertaken to comprehend the modeling techniques currently in vogue in the field of CFB. Accordingly, papers were collected and a comparative study was undertaken to understand the parameters involved and the approaches adopted [5]. It appears that the major variations among the models seem to be on the following aspects.

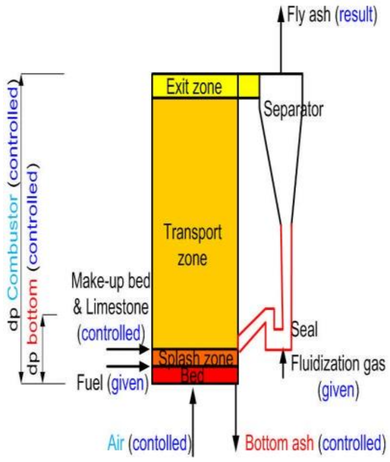

Fig 1: The circulation loop of a typical commercial CFB Boiler

A. Empirical formulations vs Use of software packages

Most of the CFB models in literature seem to be based on empirical and semi-empirical formulations. While empirical formulations seem to be mathematically rigorous and quite exhaustive, they also appear to be laborious from a designer’s perspective and scale-up appears to be a problem, especially when there are large variations in dimensions and flow parameters. Lack of adequate design techniques for scale-up of fluidized bed systems is a critical issue. Most of the current scaling techniques depend on scaling laws based on dimensional analysis or simple empirical correlations. However, they are limited to systems with predictable behavior.

State of the art computational techniques like CFD seem to have emerged as a viable alternative to such empirical models, since they appear to be more reliable in terms of scale up and predictability. CFD models are more suitable than empirical models for extrapolation or for predicting scale-up parameters from a limited amount of experimental or field data. Of the dozen software packages available, most of them are based on Eulerian Multiphase modeling. **Phoenics, CFX, STAR-CD and Fluent** are some of the known software packages that use IPSA algorithm,which can be implemented for two phase flows. Turbulence is modeled by the k-ε model. **MFIX**, developed at NETL has been widely used for CFB simulations. Syamlal O'Brien and Gidaspow models take care of solid-fluid drag correlations. Kinetic theory is handled by the modified Princeton model. **Fluent**, since its launch in 1983, has moved from single phase to multiphase modeling and is the most prevalently used code presently. Earlier versions used the IPSA algorithm. Recent versions use the phase coupled SIMPLE algorithm. Fluid- solid momentum exchange is handled by Syamlal O'Brien and Gidaspow models for granular modeling. Solid-solid momentum exchange is accounted for, by the Syamlal O'Brien symmetric model. Wen and Yu model is used for dilute system modeling. For turbulence modeling, kε model and the Reynold's stress models are employed**.**

However, using CFD codes to exclusively model and scale-up a CFB involves huge computation costs and is time consuming. More modeling ventures are being undertaken to eliminate empirical modeling and move towards computational modeling.

B. Hydrodynamics vs Other disciplines

Hydrodynamics seems to be the dominating factor in all these models, which is natural since the entire CFB flow loop is in the heterogeneous, transient flow regime, with large variations in solid–gas distribution and velocities. Quite a few papers deal with heat transfer, combustion and reaction kinetics. However, hydrodynamics is indispensable in the study of heat transfer coefficient distribution at the various sections and largely influences reaction rates due to turbulent mixing in beds.

A model frame including all the vital phenomena like combustion, gasification and emission formation in CFB boilers [6]. A three dimensional semi-empirical model, combining fundamental conservation equations, theoretical models and empirical correlations was attempted. The sub-models include fluid dynamics of solids and gases, fuel combustion and limestone reactions, comminution of solid materials, homogeneous reactions, heat transfer, sub-models for separators and external heat exchangers, and emissions. The 3D balance equations were solved for

- total gas (continuity and momentum),
- total solids,
- fuel reactions and species (moisture, volatiles, char),
- sorbent reactions and species ($CaCO_3$, CaO, $CaSO_4$, CaS, inert),
- homogeneous reactions and gaseous species (O_2, CO_2, H_2O, SO_2, CO, H_2, CH_4,C_2H_4, Cg, H_2S, NO, N_2O, HCN, NH_3, Ar, N_2),
- energy (heat transfer within suspension and to surfaces, temperature field).

The model code was written in Fortran-95 language. The visualization of the three-dimensional model results could be done either in a Matlab-application written for this model or in a generic visualization software Tecplot. The overall model results and averaged one-dimensional profiles were written to text files

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.This model provides for placement of the feeding points and heat transfer surfaces to be designed optimally [7]. The three-dimensional description of the emission formation could serve to be a very valuable tool, when optimizing the emission control. Also, the model can be applied for various troubleshooting and risk assessment studies.

An effort was made to develop a complete numerical package for heat transfer in the riser of a circulating fluidised bed boilers. It concerns the different features of the heat transfer in CFBB, namely heat transfer coefficients, temperature profiles and its dependencies on fluid dynamic and combustion models. Considering the dynamic structure of the riser, the heat transfer is present in three different fronts: from nucleus towards annulus, from nucleus towards the wall through the annulus, and directly from annulus to the wall [8]. Except for beds with low particle concentration values, convection is the dominant mechanism. For the thermal analysis, the bed is treated as an emulsion. For simplicity purpose, fundamental equations were solved using control volume analysis. The code used was written in the Matlab software. The temperature profile and heat transfer coefficients seemed to show a linear profile along the riser.

Another computational analysis of circulating fluidized bed combustion, presented coal combustion in circulating fluidized bed and the k–ϵ two-phase turbulence model was used to describe the gas–solids flow in a CFB**.** The analysis of coal combustion was done by discrete phase model (DPM) and non-pre -mixed combustion in species model. The purpose of the work was to study the char at the lower part of the furnace. GAMBIT 2.3.16 was used for making 2D furnace geometry with width of 3.2m from the lower part and height 15m. FLUENT 6.2.16 was used for analysis. Analysis was carried out for 3 velocities. It was observed that, maximum total temperature, the maximum static pressure and the turbulent intensity of the mixture, increased when the fluidizing velocity changed from 4m/s to 6m/s.

C. Drag Models

The interphase momentum transfer between the two phases represented by the drag force, play an important role in any multiphase flow approach. Due to its high relevance, this phenomenon is frequently investigated in literature. The kinetic theory of granular flow is one of the most important tools for modeling the motion of particles. The basic concept of the theory is the granular temperature. During random oscillations of the particles, inelastic collisions occur causing energy to be dissipated [9]. The granular temperature measures these random oscillations of the particles and is defined as the average of the three variances of the particle's velocities. A full mathematical description of the kinetic theory was provided by Gidaspow**.**

Since the hydrodynamics of the bed is largely dictated by the drag force exerted by the gas on the particles, several drag models have been proposed. Among the ad hoc models available, the Gidaspow model seems to be more suitable for the dense region while the Syamlal & O'Brien Model seems more suitable for the dilute region. To develop an optimum drag model, models by Gidaspow, Syamlal &O'Brien and the EMMS model were implemented into the FLUENT software and were compared by using CFD simulation [10]. An overestimation of the gas-solid drag force by the Gidaspow model and Syamlal&O'Brien models was reported. EMMS model was found to be closer in predicting the

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drag force and the dense bed formation. Efforts are on, to develop an optimum drag model by comparing the simulation results of various available drag models. Drag laws play a crucial role in quantitative and qualitative nature of segregation [11]. A more recent approach is the Energy Minimisation Multi-scale Modeling (EMMS), which looks at particle interactions in three ways:

- Micro-scale modeling of discrete particles in dilute or dense region
- Meso-scale modeling with cluster-dilute phase interaction, and,
- Macro-scale fluid particle suspension and interaction. This model has shown significant improvement in solid segregation and in predicting coarse particle behavior.

The EMMS drag model has been applied by key researchers within the field of fluidization hydrodynamics .Calculations have been made and compared for the slip velocities and drag coefficients for the different interaction phases of dense clusters, dilute phases and interactions between them both. Further, it has been proved that, a precise drag model is essential for the correct prediction of bubble formation in a fluidized bed. Since bubbles are mainly responsible for the mixing and segregation in fluidized beds, a good prediction of the bubble formation and dynamics is crucial in assessing the performance of the fluidized bed [12]. The Lattice Boltzmann drag model, used in the discrete particle model was found to predict bubble formation in a fluidized bed in a more convincing manner than the conventional drag models.

III. Component–level Models

While these are some of the obvious variants, the widest variation among the papers is seen while dealing with the flow modeling of individual components or the entire loop.

A. Reaction Bed

The CFB Combustor is characterized by its bed in which the bulk of the combustion takes place and seems to be a popular choice for modeling owing to the chaotic hydrodynamics witnessed. Good reaction rates and heat transfer rate are largely dependent upon bed hydrodynamics and modeling of fluidized bed is very crucial in scale up. Generally, the bed is divided into a dense emulsion phase at the bottom and a dilute bubbling phase at the top. A two-zone model was proposed [13- 15] to study axial solids mixing in CFB and to analyse the main specific features of the process: ascending motion of particles in the core zone and their descending motion in the annular zone (inner circulation of solids); substantial changes of particle concentration, sizes of core and annular zones over the bed height; net circulation of solids and the effect of the bottom bed on the process. The validity of the study was confirmed by comparison of calculated and experimental curves of mixing**.** Transition from bubbling to fast fluidization regime in a CFB occurs when the inlet velocity exceeds the terminal velocity. Two-dimensional and three-dimensional fluidized bed computational studies were carried out [16] to study this phenomenon**.** Fast fluidization regime is characterized by gas streaming which causes uneven fluidization. This occurrence is more relevant to petrochemical applications where FCC particles are used. 2-D and 3-D laboratory scale simulations were carried out for a bed height of 0.5m with FCC particles. The TFM model was combined with the EMMS

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drag model and used in FLUENT 6.3.26. The main focus was to explore the regimes of fluidization for a range of inlet velocities. The transition from a bubbling bed regime to a fast fluidizing regime was considered for a variety of inlet velocities in the riser of a CFB.

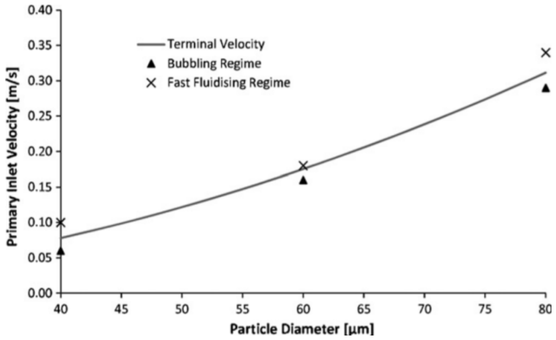

Fig. 2: Fast fluidising regimes observed above the terminal velocity, Vt, and bubbling fluidized regimes below the Vt.

Results showed that transition from bubbling to fast fluidising regimes occured after the inlet velocity exceeded the terminal velocity. Also, within the bubbling regime, bubble size was found to increase with height and so did the inlet velocity and particle diameter. The volume fraction of particles at the wall decreased with height as the particles segregated, descended and collected at the lower heights. Besides establishing the supremacy of 2-D over 3-D methods, the EMMS drag model was shown to be superior to Gidaspow drag model in addressing dilute, dense and cluster phases.

The predictions for the 2D and 3D CFB axial velocities were in good agreement with the experimental data but the 2D results slightly over predicted the core velocity. The diameter of a circulating fluidized bed (CFB) has a significant effect on the heat transfer rates to peripheral walls, a phenomenon important for the application of CFBs as combustors and boilers. Two laboratory scale models of different diameters were designed by Noymer et al. to simulate the hydrodynamic behavior [17]. To compare the effect of bed diameter on hydrodynamics, the solid-fraction profiles and the fraction of the wall covered by clusters of particles were measured. The results show that distinctly different solid-fraction profiles exist in the different-sized beds and that a 50% increase in bed diameter can nearly double the fraction of the wall covered by clusters.

A two-dimensional multi-fluid Eulerian CFD model proposed by Kuipers et al. applied the kinetic theory of granular flow to study the influence of the coefficient of restitution on the hydrodynamics of dense gas-fluidised beds. It is demonstrated that hydrodynamics of dense gas-fluidised beds (i.e. gas bubbles behaviour) strongly depends on the amount of energy dissipated in particle-particle encounters**.** It was concluded that, in order to obtain realistic bed dynamics from fundamental hydrodynamic models, it is of prime importance to correctly take the effect of energy dissipation due to particleparticle interaction into account**.**

B. Riser

The riser is characterized by large scale variations in gasparticle composition and velocities both along the axial and the radial directions of the riser.

C. Riser hydrodynamics along the radial direction

Lateral solid distribution influences particle residence time and hence reactor performance. It largely depends on inter particle collisions and interaction between particles and turbulent gas phase eddies. Quite a few earlier literature have

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proposed models for the above two mechanisms separately with moderate results. The need for a more comprehensive turbulence model was addressed by a 2-D hydrodynamic model by Nieuwland et al, which used the TFM with KTGF to model the inter particle collisions. Turbulence was modeled on a macroscopic scale, based on Prandtl mixing length model**.** Experimental validations with a cold model exposed the inadequacy of KTGF, which is based on Maxwellian steady state equilibrium conditions. Riser operating conditions deviate from this state and cannot be approximated by this assumption. Hence an under prediction of solids segregation was reported. Yet, a non-uniform radial particle distribution was established.

In the radial direction, there is a central core and a surrounding annular region. While the core is a high velocity, dilute region, the annular space can considered to be a dense, low velocity region. The usual core-annulus structure is the result of the assumption of a dilute uniform core flow, and a dense wall flow along the riser. It is attributed to the radial migration of solid flow from the wall towards the centre. However, Fan was able to establish the significant presence of a distinct wall region due to the complex dense flows at the bottom of a riser**.** A wall (boundary layer) region of dense solids concentration is developed from riser bottom because the averaged gas velocity in the wall region becomes too low to support upward moving solids. At a certain bed height, the solids in the wall region, having exhausted all their initial upward momentum, begin to move downward.

At this bed height, all solids from the upper wall region or from the lower wall region are forced to migrate inwardly towards the riser column center. At high fluidization velocities, the solids migrating inwards, mix well with the flow without reaching the centre, giving rise to the core-annulus flow.

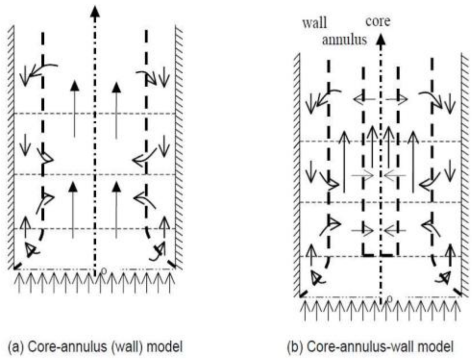

Fig 3. Radial flow segregation

At low fluidization velocities, part of the inwardly migrating solids may reach to the centerline region of riser, showing a core-annulus-wall structure. Hence, in the upper part of the riser, the solids migration into the wall causes a depletion in solids concentration. Therefore, near the top of a riser, a core-annulus-wall structure still exists but with less solids in the core than in the annulus. Modeling of both the above cases yielded the following results.

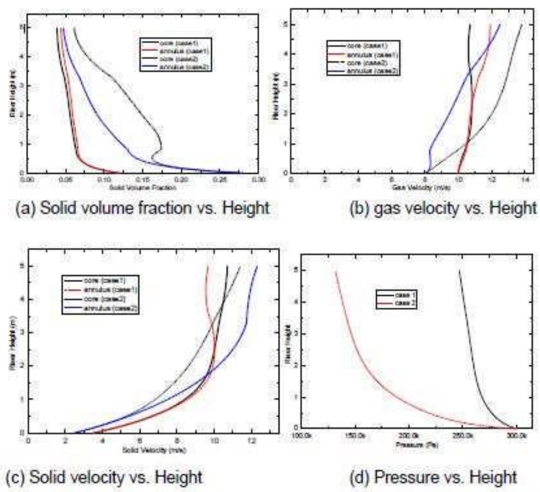

Fig.4: Variations of key hydrodynamic parameters along the riser height.

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The inhomogeneous solids distribution in the radial direction, which is unfortunately less well understood, may cause significant down flow of particles near the tube wall. The non-uniform solids distribution and solids flow influences the particle residence time distribution, and thereby the reactor performance, to a large extent. A one-dimensional model for the riser section of a circulating fluidised bed was developed by Nieuwland et al. which describes the steady-state hydrodynamic key variables in the radial direction for fully developed axisymmetric flow**.** Both the gas and the solid phase were considered as two continuous media, fully penetrating each other and empirical correlations were formulated. Gas phase turbulence was modeled using the modified Prandtl Mixing Length model. Also the effect of clusters on inter-phase momentum transfer was included. With the inclusion of a turbulence model, better predictions of axial flow velocities and radial particle distribution was obtained.
Prediction of maximum slip velocity near the wall was found in agreement with experimental values.

D. Riser hydrodynamics along the axial direction of a riser

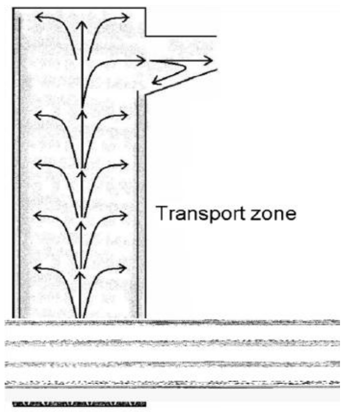

Fig.5. Zones of a CFB riser

Along the axis, the riser can be split into i) bottom splash zone ii) transport zone in the middle and iii) the exit zone based on a wide range of operating conditions like particle segregation, gas-particle velocities, etc. The inhomogeneous solids distribution in the axial direction is attributed to the acceleration of particles which enter the column at the bottom of the bed with low velocity. Factors that affect *riser bottom* operations include the condition and rate of entering solids, the arrangement of main air and secondary air inlets at the riser bottom.

Solid segregation is a phenomenon, characterized by elutriation of smaller, less dense particles by the fluidizing gas and sinking down of coarser particles to the bottom bed. Single particle 1terminal velocity is found to directly influence this segregation tendency. The Wen-Chen model, which is commonly used to simulate the elutriation and entrainment phenomena in a CFB riser, is found to be deficient in modeling the CFB combustor riser, where the flow field is characterized by fast fluidization at the top and bubbling fluidization at the bottom. In the bubbling fluidization regime, segregation depends on the interaction between the downward moving larger particles with large terminal velocities, and the gas bubbles moving upwards. Segregation in the fast fluidization zone is due to particle-particle interaction among the smaller particles with smaller terminal velocities.

A segregation model was proposed by Yao, Wang et al. for a coal combustor, based on the Cell Model, where the riser height is divided into cells. Each cell contains varied size particles exhibiting different segregation tendencies. Terminal velocity is used as the parameter influencing

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particle properties and particle interactions. Bed materials are assumed to composed of particles of constant density that have broad distribution in size, since 95% of the bed materials in a CFB boiler are coal ash. Segregation index**,** ξ, was used to describe the segregation tendency of the particles. Empirical relations were used to describe the parameters and the model was validated by conducting a mass balance of a 220 t/h CFB boiler .Good agreement between the model and experimental results were reported. The solids holdup, the length of the acceleration section, hydrodynamic mixing and transfer phenomena in risers are all influenced heavily by the riser inlet design.

The *riser exit geometry* in a circulating fluidised bed riser is shown to have a modest but consistent influence upon the particle residence time distribution in the riser of a circulating fluidised bed. Increasing the refluxing effect of the exit was shown to increase the mean residence time**.** This factor has a significant effect on the temperature distribution and scale-up. Also, its effect on solid volume fraction and velocity profile is found to influence overall pressure drop to a large extent. A predictive model by Puchyr et al. accounted for the upward flow of gas and solids in the core and downward flow of the two phases in the annulus**.** This practical model was able to adequately represent the solids mass flux and velocity profiles in a CFB operating in the fast fluidized regime. The downflow of gas and solids in the annulus, incorporated in this model, caused the average solids fraction in the fully developed zone to be altered significantly.

A further study done by Zhu et al. on particle velocity established that the solids upflowing velocity is always larger than the down flowing velocity at all radial positions, indicating that the flow of particles in the bottom region is predominantly upward through the whole cross section of the risers. And the superficial gas velocity has great influence on the solids down flowing velocity than the solids flow rate**.**

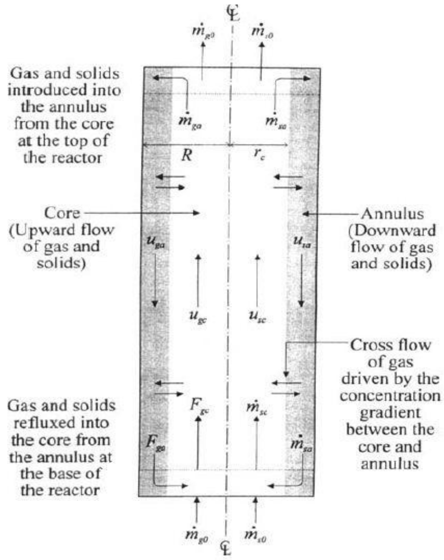

Fig. 6: Solid-gas down flow in the annulus.

Turbulence and collision are two important factors that influence cluster formation and disintegration. This aspect is important in macroscopic modeling of flow patterns in the fast fluidization regime. The k-**€** turbulence model was used in standard CFD codes are useful in modeling turbulence flow in the bed and riser**.** A steady-state model of the flow structure and mixing processes in *the upper dilute zone* of a circulating fluidized bed (CFB), where variations in flow parameters with height are neglected**,** was presented by Werther et al. The model was based on a two-phase structure, consisting of dense particle clusters and a lean gas-particle suspension as observed in several investigations. It accounted for vertical flow of gas and particles in both phases, as well as for gas and particle dispersion in the lean phase and inter-

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phase mass transfer. A 2D simulation using Fluent 6.1 was used by Hussain et al. to investigate the influence of the amount of particles on the flow pattern in the CFB system**.** The result showed the variation of velocity contours along the riser column and in the riser exit geometry. The effect was fo und to be significant in the upper region of the riser column and the velocity contours are also influenced by the exit geometry. Simulations results predicted that the riser exit caused an upstream exit region of increased solid volume fraction. Experimental and computational results are matched to reasonable agreement.

IV. Full Loop

Full loop models are yet to be developed, convincingly addressing all the decisive factors in an integrated way. An early attempt was a one-dimensional mathematical model developed by the Institute of Engineering Thermo-physics (IET) in 1996, for an atmospheric staged circulating fluidized bed boiler, taking into account the dynamics, combustion, heat transfer, pollutants formation and retention. The model of gas solid flow at the bottom of the combustor was treated by the two-phase theory of fluidized bed and in the upper region as a core-annulus flow structure. The chemical species CO, CO2, H2, H20, CH4, 02 and N2 were considered in the reaction process. The mathematical model consisted of sub-models of fluid dynamics, coal and gas chemical reactions, heat transfer, particle fragmentation and attrition, mass and energy balance etc. The model was based on the *cell model*, where the entire CFB loop was divided into cells and the mass and energy intercell interactions studied. The developed code was applied to simulate an operating staged circulating fluidized bed combustion boiler of early design and the results were found to be in good agreement with the operating data. A non-uniform temperature distribution along the furnace height was attributed to the larger size of feed coal particles and lower solid particles separation efficiency in recycle loops. The heat transfer coefficient was found to decrease with the increase in height due to reducing solids concentration and temperature along the furnace height.

It was suggested that, in order to control the temperature to meet the needs of operation safety and emission reduction in CFB furnace, the maximum size of feed coal particle should be smaller than 11 mm, and the separator efficiency in recycle loops should be further increased. On a macroscopic scale, a comprehensive semi-empirical model was presented by Pallares and Johnsson by dividing the entire CFB unit into six zones-bottom bed, freeboard, exit zone, exit duct, cyclone and downcomer and particle seal. A set of models for each of the six zones was selected and coupled in order to obtain an overall model for the entire CFB. This coupling procedure accounted for interactions between the individual zones. This model stressed the importance of a good population balance of solids for sound linking of the entire unit. Other key features that were found to be crucial in full loop modeling were, i)a set of inputs consisting only of parameters that are known and independently adjustable under operation, ii) discretization of the riser in the vertical and horizontal directions and iii)inclusion of core annulus model and the size segregation effect .

Good agreement with experimental results has been reported. Another investigation conducted a three-dimensional, full-loop, time-dependent simulation of hydrodynamics of a 150MWe circulating fluidized bed (CFB) boiler. Simulation results were presented in terms of the pressure profile around the whole loop of solids circulation, profiles of solids volume fraction and solids vertical velocity, as well as the non-uniform distribution of solid fluxes into two parallel cyclones. An Eulerian multiphase approach was used by Zhang et al. with the EMMS drag model**.** An earlier model by Witt, Perry et al. demonstrated the application of CFD to study the transient behavior in a complete fluidized system. The model was used to predict isothermal flow in a 3-dimensional bubbling bed and 2-D CFB**.**

The 3-D model showed bubble formation, with gas bubbles preferentially moving along the centre of the bed. The 2-D CFB model was able to show cluster formation and core annular flow structure. Solid recirculation was also accounted for, thus completing the loop. Inclusion of reaction kinetics of coal gasification and subsequent validation against a slug flow gasifier showed good agreement with experimental data. CFX code was used and the 2 phase Eulerian approach was adopted. To accommodate for complex geometries, a body fitted grid system was adopted. *Fuel mixing* has a great influence on the overall performance of fluidized bed (FB) combustors. Better horizontal mixing of the fuel lends a more homogenous local stoichiometric ratio over the cross section of the furnace. This would lower the occurrence of locations with un-reacted fuel or oxygen.

A high vertical mixing rate is important to ensure longer contact time between the oxygen and the fuel particles. Also, good mixing is a prerequisite for an even distribution of heat and gas release from the fuel. Pallares and Johnsson proposed that transient fluid dynamics resulting from the constantly changing physical properties of a batch of fuel particles can be used to model the fluid dynamics of a the entire loop. The mixing pattern of fuel particles, right from the instant they are injected to the bottom bed, until their recirculation in the return leg give rise to changing flow dynamics. Hence a combination of fuel particle conversion model and fuel mixing model was used to describe the entire loop hydrodynamics**.** The change in size and density of the fuel particles during conversion were used as inputs to the fuel mixing model. A 3-D model was developed and experimental validations showed a 20% deviation. Proper modeling of fuel ragmentation was found to be crucial in getting an accurate model.

V. Limitations of the current models

The Two Fluid Method (TFM) combined with the Kinetic Theory of Granular Temperature (KTGT) has been widely adopted both in empirical and CFD modeling to model both dilute and dense phases. However, this method suffers from *predictability and scale up issues.*

Assuming the particle velocity to be Gaussian and isotropic as in the TFM model, has its limitations, but the DPM method is capable of measuring the particle velocities at all locations. Further development of the single particle method combined with computational modeling tools is set to make a huge impact on the hydrodynamic modeling scenario. Another issue is the treatment of clusters, which has not been fully addressed so far. However, the recent EMMS (Energy Minimization Multi-Scale) method can be suitably coupled with computational methods to study the dynamics of clusters.

The present drag models are not able to estimate the drag forces correctly or the dense bed behavior. While the TFM methods can only relate drag coefficients with volume fractions and slip velocities, the EMMS model has been able to establish the strong dependence of drag coefficient on the structural changes. A better model which can closely predict the influence of drag on the hydrodynamics of the two phase flow will largely revolutionize modeling. Mesh independent sub-grid models are being explored which could be crucial in scaleup of CFB models. Computational modeling relies on ad hoc simulation tools to model the two-phase hydrodynamics in CFBs.

The transient nature of flow encountered in CFBs requires development of exclusive packages for transient multiphase flows. Non-availability of open source codes hinders further development. A clear idea of the range of models and correlations available is not fully known and is still largely subjective. Most of the modeling and experimental validations are specific to **FCC** reactors. More modeling ventures are required to macroscopically model the entire flow structure of CFBs and develop comprehensive models, specific to CFBs. While the flow structures are several meters high, the gas-particle interactions are confined at the micrometer levels. Empirical solutions for hydrodynamics of such large structures are not easy. Limitations on computational resource for two phase simulation (transient nature) is another bottleneck faced.

VI. Needs of CFB designers

State of the art computational methods available for simulation have made CFD models more sought after than empirical models. Despite longer simulation time and high computation costs involved, 3-d models are preferred over 2-D models. A comprehensive approach that addresses hydrodynamics, heat transfer and combustion will improve the understanding of the full loop dynamics. A suitable hybrid model that combines the existing Euler-ian and Lagrang -ian model combined with a modified drag model like the EMMS model could revolutionize the modeling approach. The MPPIC , which combines the advantages of both models, hold promise in future modeling. A parcel based, full loop, CFD modeling approach is predicted to take over in the near future, thereby eliminating experimental validations.

VII. Conclusion

A good CFB model is expected to predict some or all of the following: bed expansion, gas flow pattern, solid flow pattern, bubbling size /frequency / population, 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, back mixing and down-flows in risers and solids distribution/segregation. More modeling efforts along these lines could lead to the evolution of better models with better convergence for the entire CFB loop. That is what a designer wants.

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