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CFD SIMULATION SCALE-UP OF A DUAL-FLUIDIZED BED GASIFIER FOR BIOMASS

Anjani Kumar DIDWANIA and Robert J. CATTOLICA

Department of Mechanical and Aerospace Engineering,

University of California, San Diego, La Jolla, Ca, 92093-0411, USA

ABSTRACT

The University of California in collaboration with West Biofuels, LCC, has developed an advanced thermo-chemical gasification system (5 ton/day) for the conversion of waste stream biomass for the production of bio-fuels and bio-energy. The "Pyrox" gasifier design is based on a dual-fluidized bed system operating at atmospheric pressure with air. Simulation of this gasifier was conducted with a new CFD simulation software package, SDBG (San Diego Biomass Gasifier), developed from the open source MFIX code from the National Energy Technology Laboratory as its kernel.

SDBG was used to perform CFD simulation of the gasifier column reactor with its detailed geometry in full size and at 1/5 scale for two sets of mono-disperse particles of differing size and density. It is often assumed that dynamic similarity can be ensured only when the Glicksman's full set of non-dimensional scaling parameters are kept identical. However, CFD simulations suggests that Glicksman's much desired simplified set of scaling parameter suffices for dynamic similarity as long as the particle collision properties (particle-particle and particle-wall restitution coefficient) used in continuum kinetic theory closures are kept at a critical value.

Keywords: Fluidization, Scale-up, simulation, Biofuels, Biomass, Gasifier, CFD, SDBG, PYROX

NOMENCLATURE

d_p Particle Diameter
D Bed Diameter
e Particle-particle restitution Coefficient
F_i Interaction Force

$$F = \frac{u_o^2}{gd_p}$$

g Acceleration due to gravity
G Pressure Fluctuation Transfer Function
H Bed Height
p^s Solids Phase Pressure
p^f Gas Phase Pressure
P Pressure Power Spectrum

$$Re = \frac{\rho^s d_p u_o}{\mu^f}$$

$$R = \frac{\rho^f}{\rho^s}$$

T Granular Temperature
u_i Particle phase velocity
u_o Gas Phase velocity in Max. Diameter Section
v_i Particle phase velocity
ρ^f Gas density
ρ^s Solids density
η^f Gas shear viscosity
η^s Solids shear viscosity
ζ^f Gas bulk viscosity
ζ^s Solids bulk viscosity
ω Angular Frequency
ω_n Characteristic Angular Frequency
ξ Damping Constant
σ statistical variance of white noise input
σ_{ij}^s Solids Phase Stress
σ_{ij}^f Gas Phase Stress
λ Granular Conductivity
ϕ Particle Concentration
Γ_s Particle Fluctuating Kinetic Energy Source
Γ_d Particle Fluctuating Kinetic Energy Sink

INTRODUCTION

In biomass gasifiers, the flow is complex given the heterogeneous nature of the particles, turbulence of the fluidizing fluid, complex geometries, simultaneous heat and mass transfer, and rapid gas release during devolatilization. In addition, the gasifier involves biomass particles co-fluidized with much denser and more regular bed particles such as sand. Interaction and mixing of the species then become major issues. Currently, there are no published general rules or principles helpful in understanding multiphase flow in biomass gasifiers. The few existing reports [Rao et al. (2001), Lv et al. (2004)] on biomass fluidization deal primarily with topics like minimum fluidization velocity, ways of achieving fluidization, mixing and segregation, and residence time distributions. These works treat mostly low-velocity fluidized beds and often inert particles to model biomass. In actual systems however biomass particle are mixed with inert bed particles like sand and even at times catalyst materials are introduced. Further research is needed to provide a general understanding of the interactions among heterogeneous particles and guidance on conditions most likely to lead to viable and sustainable processes.

The University of California in collaboration with West Biofuels, LCC, has developed an advanced thermo-chemical gasification system for the conversion of waste stream biomass (forest waste, agricultural waste, and urban green waste) for the production of biofuels and bioenergy.

Fig.1 UC Discovery/West Biofuels 5 ton/day dual-fluidized bed reactor based on the "Pyrox" design at the West Biofuels, Woodland Biomass Research Centre in Woodland, CA

The "Pyrox" design is based on a dual-fluidized bed system operating at atmospheric pressure with air as illustrated schematically in Fig 2.

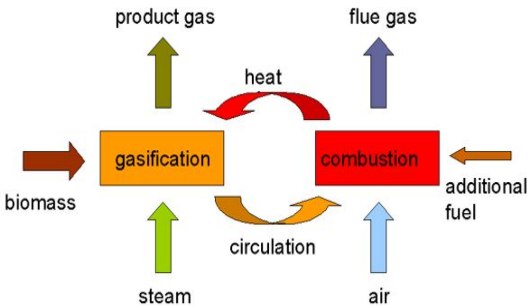


Fig.2 Pyrox design Schematics.

In dual-bed gasification the biomass is introduced in a reactor where volatiles and some fixed carbon are converted to product (producer) gas in the presence of steam. The bed material in the gasifier carries the remaining fixed carbon (char) to the combustion section of the dual-fluidized bed where air is introduced for combustion and energy is released to heat the bed, which is returned to the gasifier reactor through re-circulation of the bed material. Critical to the commercial success of the less expensive dual-fluidized bed gasifier is the ability to understand and control the fluid dynamic/chemical kinetic processes for gasification and to have a reliable engineering design tool to scale research and pilot scale (~ 150 tons/day) systems to large commercial scale (~1500 tons/day). The development of an advanced computation fluid dynamic (CFD)/chemical kinetic model for the dual-fluidized bed gasifier is therefore an essential element in moving the technology from laboratory and pilot scale to commercialization. CFD is undergoing significant expansion in terms of its applications in various chemical processes, involving the numerical solution of conservation equations for mass, momentum and energy in all flow geometry of interest, together with additional sets of equations reflecting the problems at hand, e.g., reacting flows. Basic mechanisms are included in the governing equations, which bring a great advantage to CFD, i.e., once a CFD model is validated by experimental data and accepted as a reasonably accurate description of processes in a reactor, it can be used for scale-up and design.

Application of these CFD codes to biomass gasifiers utilizing bubbling bed and circulating fluidized bed reactors is reviewed previously [Dimitrios et al. (2001)]. To converge on an appropriate computational simulation approach for our modeling, design and optimization of UC/West Biofuel Reactor, preliminary computational studies were conducted using both the commercial software Fluent and open source software MFIX from NETL on simple fluidization geometries. Based on the results of this preliminary study, the MFIX code from NETL was chosen as the kernel for a new biomass gasifier simulation package named as the San Diego Biomass Gasifier (SDBG). The choice of MFIX was primarily based on accessibility to the source code and reported success of MFIX in simulating transient three-dimensional simulations with chemistry and heat transfer of an industrial scale Kellogg Brown & Root, Inc. (KBR) Transport Gasifier in operation at the Power Systems Development Facility (PSDF) in Wilsonville, Alabama (Guenther et al. 2003). Since the UC/West Biofuels Biomass gasifier has many features in common with the fossil fuel gasifier at PSDF, MFIX code was adapted in SDBG for simulating the fluid dynamics and chemical kinetic for biomass gasification and the generation of producer gas. The set of modeling equations underlying SDBG package are essentially similar to those used for MFIX.

Scaling and Dimensional Analysis

Because basic measurements on a full-size commercial reactor are often prohibitively complex and expensive, the hydrodynamics of a large commercial unit is usually mimicked by using a lab-scale model. However, due to the complicated phenomena encountered in most multiphase flow systems, fluidized bed reactor scale-up is extremely difficult to this date. Combining CFD with similitude methods and selected experimental study could be an efficient way to facilitate the scale-up, design and operation of a multiphase process.

Buckingham π-theorem and non-dimensionalization of governing equations have been used in the past to produce sets of dimensionless parameters which are kept constant to achieve dynamic similarity. Fitzgerald and Crane (1980) used the Buckingham π-theorem approach to deduce the scaling parameters as the Reynolds number, the density ratio, the Froude number, bed to particle diameter ratio and geometrical similarity of the beds. Glicksman (1994) obtained a similar set of scaling parameters ("full set") by non-dimensionalizing mass and momentum conservation equations for both phases given as

$$\frac{u_0^2}{gd_p}, \frac{\rho^f}{\rho^s}, \frac{\rho^f u_o d_p}{\eta^f}, \frac{H}{D}, \frac{D}{d_p} \tag{1}$$

By assuming a relationship between slip velocity and particle terminal velocity, he showed that this full set can be reduced to simplified sets depending on the nature (viscous/inertial) of the flow regime, as for example,

$$\frac{u_0^2}{gd_p}, \frac{\rho^f}{\rho^s}, \frac{\rho^f u_o d_p}{\eta^f}, \frac{H}{D} \tag{2}$$

It is to be noted that in his derivation, Glicksman ignored particle phase stresses and conservation of particle kinetic energy fluctuation equation and thus he was unable to account for particle kinetic energy collisional dissipation and exchange effects in the set of scale-up parameters.

Detamore et al. (2001) used a kinetic-theory model to investigate the validity of various sets of scaling laws for CFB configurations. Their work shows that properties of particle collisions must be included to ensure similarity. They also observed that detailed hydrodynamics similitude is not achieved for reduced scaling sets in which the ratio of the particle diameter to tube diameter is omitted. It may however be noted that their study is limited only to fully-developed (only radial variation allowed) tube flow fluidization. Van Ommen et al. (2006) find computationally that Glicksman's full set gives the largest differences for scale-up whereas the simplified set performs better, but neither leads to complete similarity. Their study, however, used a constant value of particle-particle restitution (e=.95) and didn't analyze its effect on similitude. A systematic study of scaling effects with CFD to identify the complete set of scaling parameters including as yet unidentified potentially active dimensionless groups especially those due to particle stress, particle kinetic energy fluctuation source and collisional dissipation effects, remains to be undertaken.

The objective of the present simulation scale-up study is to identify the relevant scaling parameters for Pyrox design of biomass dual bed gasifier using the SDBG simulation package. We report here a comparison of the simulation results for the full scale gasifier column in the dual fluidized bed with its 1/5th scale model for a set of relevant scaling parameters under bubbling fluidization conditions. In what follows, we describe the simulation model, the simulation procedure followed by the results and the conclusion.

MODEL DESCRIPTION

The SDBG (San Diego Biomass Gasifier) simulation package, like MFIX, is developed mostly within a multi-fluid framework (also referred to as Eulerian-Eulerian model). In a gas-solids system with mono disperse solids, the hydrodynamic model treats the fluid and solids as two continuous and fully miscible phases. This approach results in mass, momentum, and energy balance equations for each of the two phases separately. The governing conservation equations for the dispersed two phase system in cold flow with no chemical reactions can be reduced to the following form (Didwania 2000, Didwania 2001)

Continuity:

$$\text{Particle}: \frac{\partial \phi}{\partial t} + \frac{\partial \phi v_i}{\partial x_i} = 0 \tag{3}$$

$$\text{Fluid}: \frac{\partial (1-\phi)}{\partial t} + \frac{\partial (1-\phi) u_i}{\partial x_i} = 0 \tag{4}$$

Momentum:

$$\text{Particle}: \rho^s \phi [\frac{\partial v_i}{\partial t} + v_j \frac{\partial v_i}{\partial x_j}] =$$

$$\frac{\partial \sigma_{ij}^s}{\partial x_j} + F_i + \phi \rho^s g_i \tag{5}$$

$$\text{Fluid}: \rho^f (1-\phi)[\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j}] =$$

$$\frac{\partial \sigma_{ij}^f}{\partial x_j} - F_i + (1-\phi)\rho^f g_i \tag{6}$$

Particle Phase Granular Temperature:

$$\frac{3}{2}\rho^s \phi (\frac{\partial T}{\partial t} + v_j \frac{\partial T}{\partial x_j}) =$$

$$\sigma_{ij}^s \frac{\partial v_i}{\partial x_j} + \frac{\partial}{\partial x_i}(\lambda \frac{\partial T}{\partial x_i}) + \Gamma_s - \Gamma_d \tag{7}$$

For both phases assumed to be newtonian, the phase stresses are given as

$$\sigma_{ij}^f = -p^f \delta_{ij} + \zeta^f \frac{\partial u_k}{\partial x_k} \delta_{ij} + 2\eta^f D_{ij} \tag{8}$$

$$\sigma_{ij}^s = -p^s(\phi, T)\delta_{ij}$$

$$+\zeta^s(\phi, T)\frac{\partial v_k}{\partial x_k}\delta_{ij} + 2\eta^s(\phi, T)S_{ij} \tag{9}$$

where

$$S_{ij} = \frac{1}{2}(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} - \frac{1}{3}\frac{\partial v_k}{\partial x_k}) \tag{10}$$

and .

$$D_{ij} = \frac{1}{2}(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{1}{3}\frac{\partial u_k}{\partial x_k}) \tag{11}$$

Closure expressions for p^s, ζ^s, η^s, λ, Γ_s, Γ_d used in the simulations are derived from kinetic theory of granular flows and are given in MFIX documentation (Benyahia et. al. 2005). The interaction force F_i includes drag and buoyancy terms. There are several gas/particle drag models for the drag terms. The present simulations are performed with two different drag models proposed by Syamlal and O'Brien (1987) and Wen and Yu (1966). Expression for Γ_d, particle fluctuation energy dissipation term contains e, the particle-particle restitution coefficient which influences simulations significantly. The restitution coefficient e (both particle-particle and particle-wall) is a measure of kinetic energy dissipated in collisions with e=1 representing elastic collision. It is a continuum measure of collisional dissipation related to individual particle-particle collision only in an averaged sense. At the wall, Johnson and Jackson (1987) boundary condition is applied for the solids phase with the particle-wall restitution coefficient kept fixed at .85 for all simulations reported here. This value was chosen to keep the particle-wall restitution coefficient in the same range as the particle-particle restitution coeffiecient. A detailed study of particle-wall restitution coefficient effect will be reported elsewhere.

Procedure

SDBG simulation package was used to perform CFD simulation of the gasifier column with its detailed geometry in full size and at 1/5 scale for two sets of mono-disperse particles of differing size and density. The full gasifier column is 8.75 m tall with variable diameter in the range of minimum .2 m at the inlet and top and a maximum of .6 m in the upper section. The 1/5th scale gasifier is geometrically similar to the full scale. The initial bed height was taken as 2.5 m for the full scale gasifier and .5 m in the 1/5 scale to maintain similarity. Fluidization of two mono disperse particle sets (Table 1) are simulated.

Particle set	d_p in cm	Specific Gravity	d_p / D (full)	d_p / D (1/5)
Set A	.0425	3.56	.00213-.00639	.01065-.03200
Set B	.0334	2.7	.00167-.005	.00835-.025

Table 1. Particle Sets in Simulation

Table 1 shows the min-max range for d_p / D in each of the gasifier columns. Since it is a column of variable diameter, the minimum fluidization velocity is not uniquely defined. The simplified scaling parameter set is adopted by keeping constant the three dimensionless parameters at Fr=15, Re=30 and R =.0003 in all simulations. The dimensionless numbers are defined with respect to the fluidizing gas velocity in the maximum diameter section of the column. This leads to variation of fluid velocity in the variable diameter columns.

Numerical method employed for time discretization is implicit backward Euler method and for the convective terms discretization is superbee or first-order upwind. The set of non-linear equations is linearized using a modified version of the SIMPLE (Patankar, 1980) algorithm using void fraction and gas pressure correction equations. The resulting system of sparse, non-symmetric linear equations for each of the equations is solved using the algorithm by Barrett et al. (2006). Details are similar to that available in the MFIX numerical guide (Syamlal, 1998). After a detailed numerical investigation, optimal grid resolution and discretization schemes were selected. Since the bed is of variable diameter, the long inlet region is essentially single phase fluid flow with a bubbling fluidized bed confined mostly in the middle region. Hence the grid resolution is kept variable with square cells in the radial-axial direction having maximum size 4 mm. There are 10 cells in the circumferential direction. A second order discretization scheme has been used for the results reported here.

To examine dynamic similarity between full and 1/5 scale simulation, we adopt the now well-recognized technique of comparing pressure fluctuation in frequency domains (Falkowski and Brown, 2004). Scaling parameters in bubbling fluidized beds have been tested in experiments by monitoring pressure fluctuations as an indirect measure of bubbling phenomena. Usually the pressure fluctuations are characterized by a single, dominant frequency and this frequency matching is used to compare scaling parameters. In recent years for better comparison, the pressure fluctuations are increasingly viewed as a broadband phenomena arising from the output response of a dynamical system (the fluidized bed) to an input disturbance. A bubbling fluidized bed can be well-represented as two second order dynamical system in parallel (Bi, 2007). Bode plots are then employed to evaluate pressure data from fluidized beds. A Bode plot is a logarithmic graphical representation of power spectral density as a function of frequency where the pressure spectral density function $P(i\omega)$, is calculated from time series data and is expressed in terms of the complex transfer function, $G(i\omega)$ as

$$10\log P(i\omega)=20\log|G(i\omega)|-20\log\sigma. \qquad (12)$$

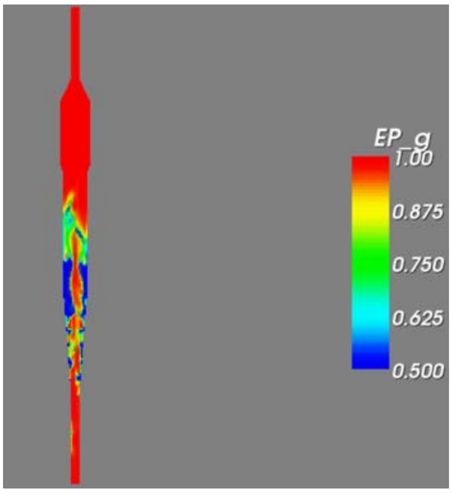
For second order representation of bubbling fluidized beds. $G(i\omega)$ is (Falkowski and Brown, 2004)

$$G(i\omega)=\frac{1}{\left(1-\frac{\omega^2}{\omega_{n1}^2}\right)+i2\omega\left(\frac{\xi_1}{\omega_{n1}}\right)}+\frac{1}{\left(1-\frac{\omega^2}{\omega_{n2}^2}\right)+i2\omega\left(\frac{\xi_2}{\omega_{n2}}\right)} \qquad (13)$$

By plotting $|G(i\omega)|$ vs. ω and evaluating the characteristic frequencies, ω_n, and damping constants, ξ, pressure fluctuations in two bubbling fluidized beds can be compared to test the scaling parameters.

Results

The fluidization quality in the gasifier column is illustrated in Figure 3. Since the ratio of maximum to minimum diameter in the column is three, solids in the bottom section of the column are in pneumatic transport while fluidization of the upper section is in freely bubbling state. Figure 4 illustrates typical pressure fluctuation in the centerline of the bed in the middle 20 inch diameter section of the bed.



Fig, 3. A vertical section snapshot of dynamic simulation of the full gasifier column at steady state. (Table 2, Set A: d_p / D = .00639, e=.85) The colour scheme for gas void fraction EP_g gives void fraction in the bed.

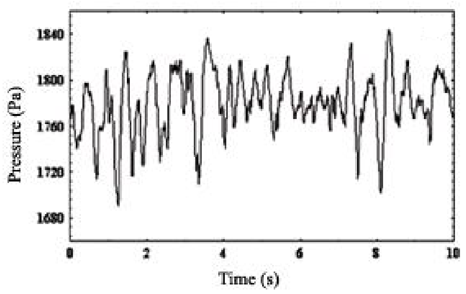


Fig. 4. Typical Pressure Fluctuation Profile in Full Scale Bed Simulation

Comparison between the full and the 1/5th scaled model is achieved by fitting the transfer function G(iw) to the Bode plot of pressure fluctuations. The fitted constants are presented in Table 2. This Table corresponds to the case of particle-particle restitution coefficient, e=.85 where we find an excellent agreement between scaled beds for best-fit characteristics frequencies and damping constants. As the e value is changed, there is less agreement between the fitted constants corresponding to full and the scaled model as shown in the next Table.

particles	Size	d_p / D	ω_{n1}	ω_{n2}	ξ_1	ξ_2
Set A	Full	.00639	2.4	4.1	.40	.46
Set A	1/5	.03200	2.38	4.20	.39	.45
Set B	Full	.005	2.39	4.15	.41	.44
Set B	1/5	.025	2.4	4.15	.40	.44

Table 2: Comparison of Characteristic Frequencies and Damping Constants for e=.85 for Full and 1/5 scale model

particles	Size	d_p / D	ω_{n1}	ω_{n2}	ξ_1	ξ_2
Set A	Full	.00639	1.2	4.9	.4	.31
Set A	1/5	.03200	1.6	4.0	.5	.52
Set B	Full	.005	2.8	3.0	.35	.45
Set B	1/5	.025	2.1	5.0	.39	.61

Table 3: Comparison of Characteristic Frequencies and Damping Constants for e=.80 for Full and 1/5 scale model

CONCLUSION

Simulation results suggest that under geometrical similarity for mono disperse particles, a simplified set of scaling parameters (three dimensionless parameters) along with a critical value of particle restitution coefficient is sufficient to maintain dynamic similarity between the full and 1/5 scale model of the gasifier. Variation in d_p / D ratio does not affect scaling agreement even though diameter of the gasifier column varies over a ratio of 1 to 3. This observation is different from both of earlier CFD simulation studies. While Detamore et al. (2001) determined d_p / D to have significant influence and recommended using "full-set" in addition to particle-particle restitution coefficient, Van Ommen et al. (2006) observed that simplified set performs better scaling. Our observation of existence of a critical value of particle-particle restitution coefficient for scaling similarity emphasizes a need for further exploration of unidentified dimensionless scaling variables based on the analysis of particle kinetic energy fluctuation conservation equation and subsequent CFD simulations. In addition, while dynamic similarity has been defined in the present context via frequency spectra of pressure fluctuations, matching of void fraction, phase velocity and pressure profiles can be equally important in scale-up considerations.

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