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COMPARISON OF ENTRAINMENT RATE IN ACRYLONITRILE REACTORS USING PLANT DATA AND CFD SIMULATIONS

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ABSTRACT

Accurate entrainment rates are important in fluidized bed reactors for several reasons, including determination of cyclone loadings and efficiencies, sizing of diplegs, and inputs to population balance models. Entrainment correlations exist in the literature and from other sources to predict entrainment rates from fluidized beds, but they can vary by orders of magnitude. In addition, many correlations do not take into account effects of internals which are present in many types of industrial reactors. A study was undertaken to better understand entrainment rates from Sohio-type acrylonitrile fluidized bed reactors containing catalyst classified as a Geldart type A powder. As part of this study, full scale CFD models were developed using the Barracuda® computational particle fluid dynamics (CPFD®) software and validated with the help of data collected from multiple plant reactors. These models compared two different sizes of industrial-scale reactors and included all major internals including cooling coils, cyclones, cyclone diplegs and gas spargers.

Data on the pressure profile and actual entrainment rate to the cyclones generated by the Barracuda models were compared to the measured pressure data and derived entrainment rate in the plant reactors. The results showed good agreement. Additionally, evaluation of using the slip factor in the model to compare the particle volume fraction in the freeboard to the actual entrainment rate was done to determine if this technique could be used in the plant setting. The slip factor as calculated by Barracuda was between 1.55-1.95 which is similar to other values in the literature.

INTRODUCTION

Barracuda® CPFD model pressure profiles and entrainment rates were compared to plant reactor data from two different diameter Acrylonitrile reactors. In the industrial setting, accurate entrainment rates are important in fluidized bed reactors for several reasons, including determination of cyclone loadings and efficiencies, sizing of diplegs, and inputs to population balance models. Entrainment correlations exist in the literature and from other sources to predict entrainment rates from fluidized beds, but they can vary by orders of magnitude. In addition, many correlations do not take into account effects of internals which are present in many industrial reactors. In contrast, a full-scale Barracuda model can take into account effects of particle size distribution and effects of internals and reactor walls. In addition to the direct Barracuda model predictions, the idea of using a slip factor applied to actual plant reactor pressure measurements in the upper freeboard near the cyclone inlets was explored within the model. This technique may provide a simplified way to more directly estimate entrainment rates in industrial reactors.

REACTOR SYSTEM

The two reactors studied were Sohio-type Acrylonitrile reactors, as illustrated in Figure 1. These reactors are described by Kunii and Levenspiel (1) as having a uniform air feed through a bottom distributor and an upper distributor where ammonia and propylene are fed. The Sohio reactors have numerous vertical coolant coils that circulate water and produce steam from the highly exothermic reaction. Internal cyclones collect the catalyst from the effluent gas and return it to the bottom of the reactor.

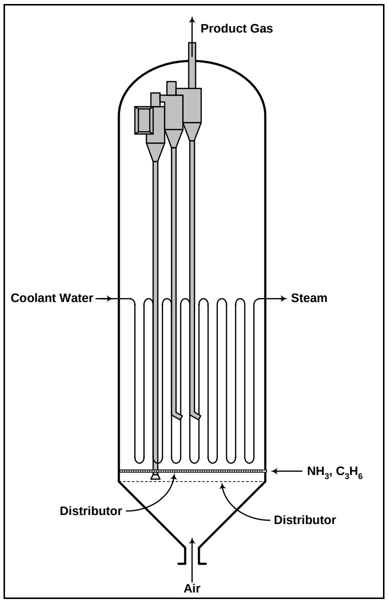


Figure 1. Sohio-type Acrylonitrile Reactor, Modified from Kunii and Levenspiel (1)

Table 1. Operating and Model Conditions

Catalyst $d_{p\ 50}$, microns	50-65
Fines Content, < 44 microns	10-35
Particle Density, kg/m^3	1400-2000
Reactor Diameter, m	3.6 (small), 9 (large)
Operating Pressure, kPa	100-200
Operating Temperature, °C	425-490

Pressure profiles were taken with local digital pressure gauges. Due to the limited nozzle locations on the reactor vessels, the pressure profile was limited to approximately ten locations along the reactor height. The pressures were taken at points approximately 1 foot from the wall of the reactor vessels using internal piping.

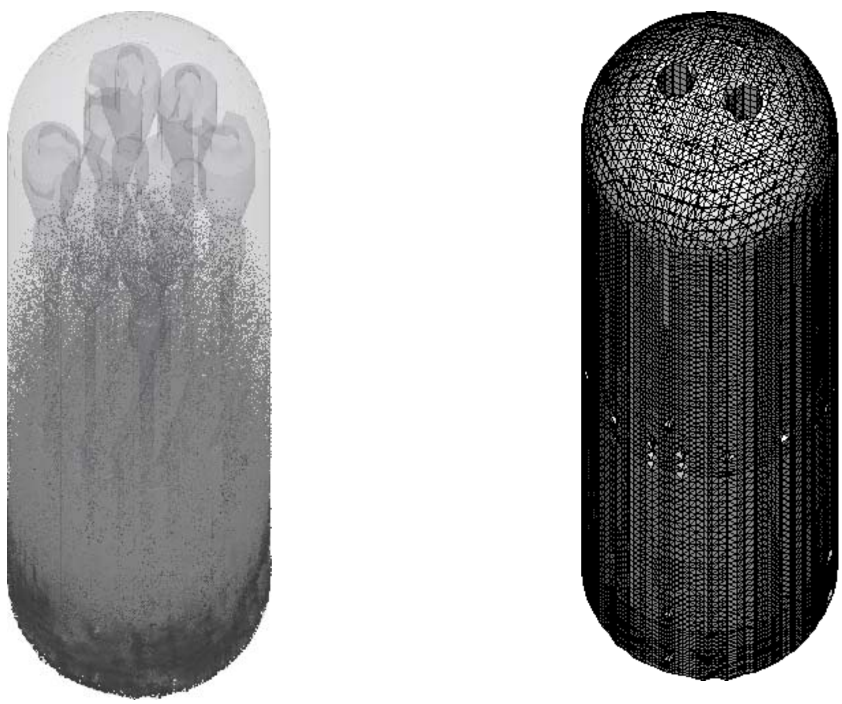
NUMERICAL MODEL (CPFD)

The three-dimensional gas-solids flow inside the two Acrylonitrile reactors operating in the turbulent fluidization mode was numerically simulated using the commercial Barracuda software package. The Barracuda software is an advanced math-physics based numerical tool built on the technology of the computational particle-fluid dynamics (CPFD) developed by CPFD Software. The software's numerical methodology uses a direct element method where solids are modeled using the Lagrangian method as discrete particles with proper size and density distributions, and the fluid is modeled as a continuum solved on a fixed grid using the Eulerian method. The actual solids particles numbering in the order of 10^{15} to 10^{18} are typically modeled with 1 to 5 million numerical particles, each of which groups the physical particles with the same properties (size, density, etc) as a single entity. Each of the numerical particles is explicitly tracked and calculated for its position and motion in the Lagrangian scheme. Solutions of the fluid dynamics and solids motion and their interaction are fully coupled. The software has been extensively validated against available theoretical and experimental data, and it is efficient in simulating large commercial scale fluidization units.

The reactor simulations included all major internals including cyclones, diplegs, cooling coils and support beams and gas spargers in the numerical model. Figure 2(a) shows the larger reactor loaded with solids particles. The reactor model was discretized with approximately 200,000 cells. A quarter of the gridded model cutting through the center lines is shown in Figure 2(b). The geometry of the smaller reactor was similar with fewer cyclones and coils.

The simulation conditions are typical operation conditions of Acrylonitrile reactors. Since fluidization behavior of the bed was the focus of the study, chemical reactions and thermal dynamics and heat transfer were not considered. The fluid, a gas mixture of air and hydrocarbons, had a superficial gas velocity of approximately 0.6 m/s. The reactor was initially loaded with solids particles at near close-pack volume fraction. The flow boundary conditions included fluidizing gas entering the bed uniformly through the bottom of the reactor and through the gas sparger at a higher elevation inside the reactor, pressure boundary conditions at the cyclone inlets where gas and solids flow exit the system, and solids returned to the bed through the bottom of the primary and secondary diplegs. The rate of solids returned to the bed from the diplegs matched approximately the rate of solids entrainment through the cyclones so the bed inventory was maintained almost constant during the simulation. The variation of bed inventory is within 1~2%. A typical simulation was approximately 200 s of real-time operation; about 100s to reach quasi-steady state and an additional 100 s is run to obtain average properties such as the particle volume fraction, the pressure and gas and solids velocities.

Two simulations were performed on different reactor sizes both with a superficial gas velocity of about 0.6 m/s.



(a) (b)

Figure 2. One of the Two Acrylonitrile Reactors Simulated. (a) The Whole Reactor with Solids Particles Being Fluidized at the Early Stage of the Simulation. (b) Gridded Model.

RESULTS AND DISCUSSION

Pressure vs. Elevation

Pressure vs. elevation as well as density vs. elevation were measured in the plant and computed by the Barracuda model and were compared in Figures 3-4. The key parameters of the Barracuda models and the plant reactor were chosen to be as close as possible for a good comparison. They are shown on a relative basis to the maximum elevation and pressure. In addition, calculated points corresponding to the relative top pressure accounting only for the weight of the bed as well as the relative top pressure using the bed weight and correcting for an average 6% reduction in cross-sectional area due to the reactor internals are shown for comparison..

From Figures 3, the Barracuda pressure vs. height shows a more gradual decrease in pressure than the plant data. The model shows reasonably good agreement with the pressure survey data over the entire reactor height. A force balance check showed that the pressure drop calculated by the Barracuda model matched the bed weight within 5%.

Figure 4 shows the pressure profile of the 3.6-meter diameter reactor compared to the pressure profiled predicted by the Barracuda model. In this case, the pressure profile matched the shape of the plant data closely up to about 40% of the reactor bed height. The top point of the plant reactor survey shows about 2% difference from the Barracuda model. While the overall inventory in the model matched the plant within 5%, the pressure deviation may be due to de-fluidized catalyst in the plant reactor and catalyst below the bottom pressure tap that is not contributing to the overall pressure drop.

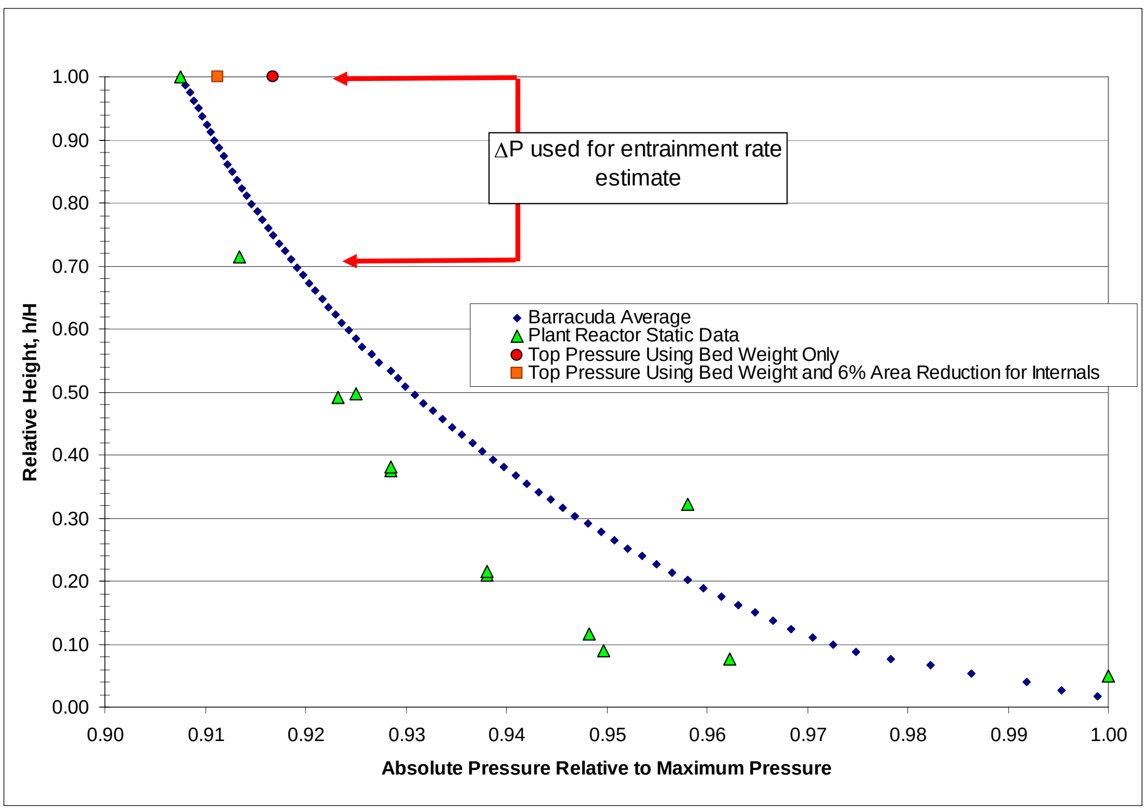


Figure 3. Pressure Profile Comparison in the 9-m Diameter Reactor

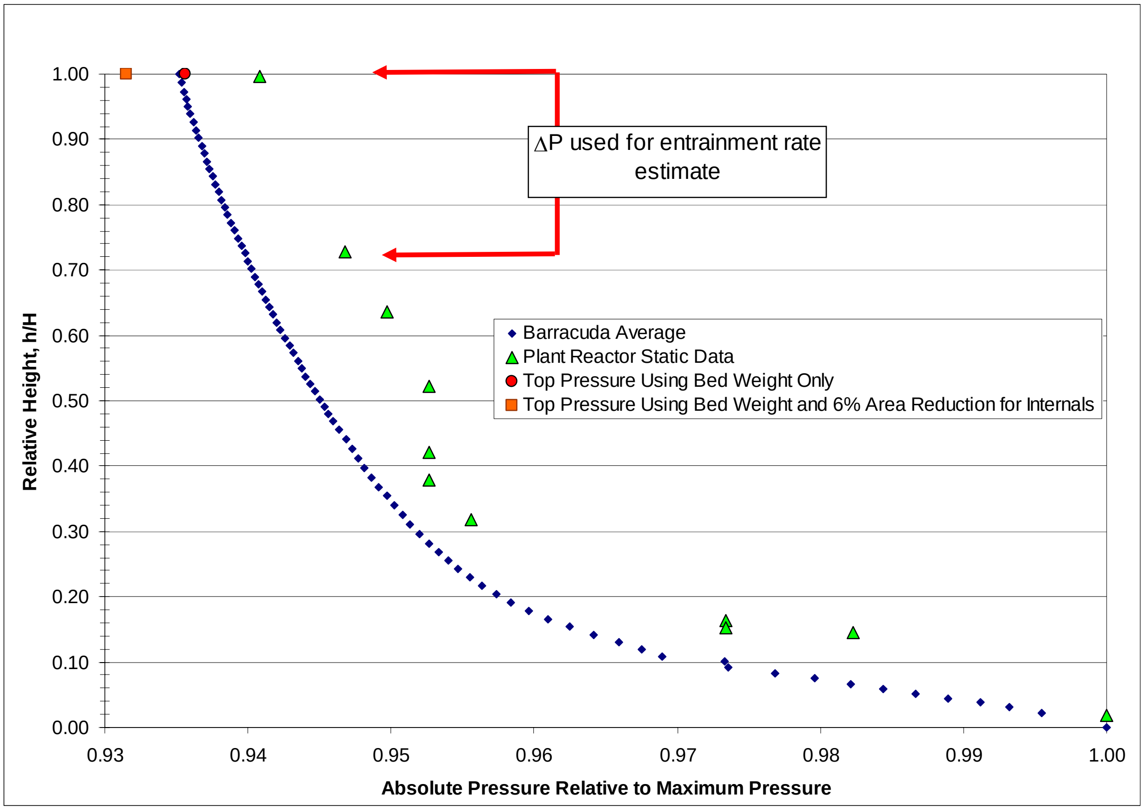


Figure 4. Pressure Profile Comparison in the 3.6-m Diameter Reactor

Entrainment Rate Comparisons

One of the key parameters desired from the pressure survey and the Barracuda models was an estimate of the entrainment rate of solids to the cyclones. While the upper limit of the entrainment can be calculated from the upper-most bed density, the actual entrainment to the cyclones would be lower. A question posed during this study was if a slip factor could be applied to the upper-most bed density to better estimate the entrainment rate and cyclone loading. The slip factor, as defined by Patience, *et.al.* (2), is the ratio of the gas velocity to the particle velocity. In parallel, the Barracuda model offered a way to not only apply this concept within the model, but to also directly compare to the actual entrainment with the model itself.

$$\psi = U_o/(\varepsilon_{avg}V_p) \quad (1)$$

The average particle velocity is calculated from Eq. (2) and the voidage from Eq. (3) assuming pressure drop is only due to the hydrostatic head of the solids:

$$V_p = G_s/[\rho_p(1-\varepsilon_{avg})] \quad (2)$$

$$\varepsilon_{avg} = 1- dP/(\rho_p g dz) \quad (3)$$

The slip factor defined by Eq. (1) was directly calculated from the Barracuda simulation. Figure 5 shows the slip factor for both reactor diameters at various elevations over the equivalent range between the top two pressure taps in the plant reactors. The slip factor was 1.47 to 2.97 over this elevation range. The 9-m reactor average slip factor was higher than the 3.6-m reactor which was also reflected in the higher predicted entrainment rate shown in Table 3. The arithmetic average slip factor around 2 indicated that on average the particle velocity was less than half of the fluid velocity (note that the average void fraction was around 0.97). Due to the difference in the particle and fluid velocities, the actual entrainment rate was much less than that calculated under the assumption that the particle and fluid flow to the cyclone together at the same velocity. The Barracuda simulation predictions match well with data from Patience, et. al. where the slip factor in the fully developed region of CFB risers from various data sources was calculated as approaching 2. The entrainment flux (G_s) from the acrylonitrile reactors was calculated from Equations 1 to 3 using the average Barracuda model calculated slip factor applied to the top most differential pressure measurement under the operating conditions present.

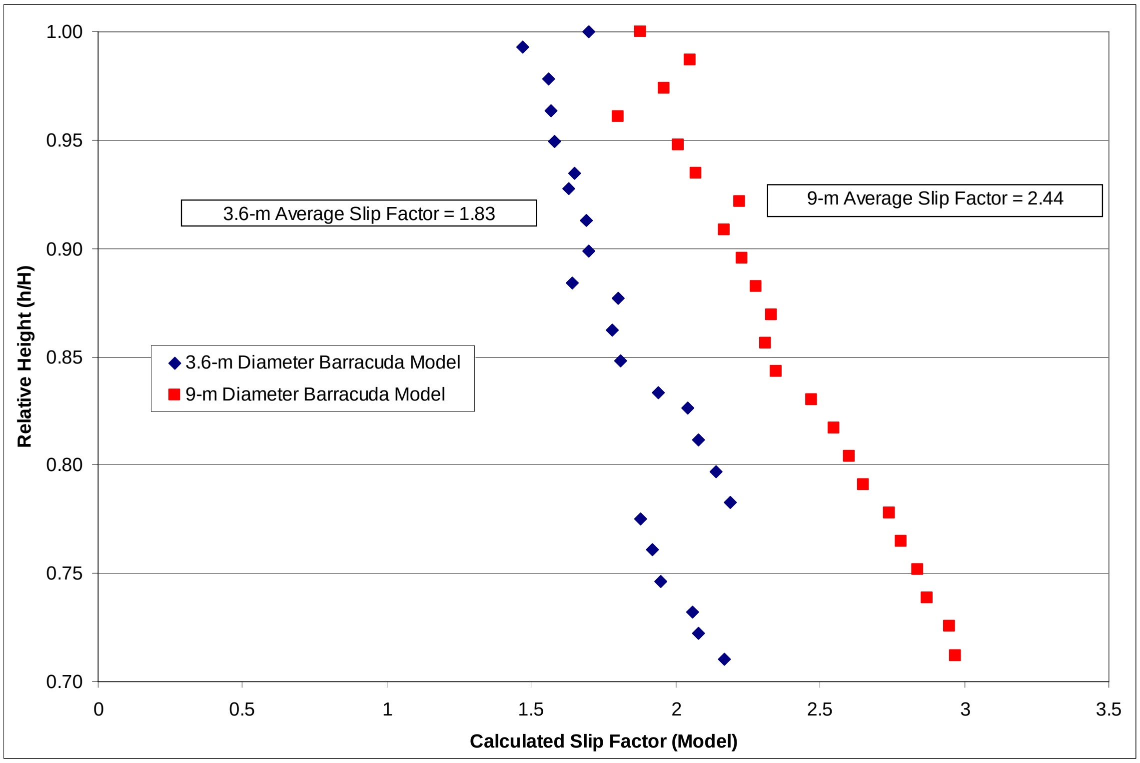


Figure 5. Slip factor calculated by Barracuda at elevations between the top two plant reactor pressure taps

The Barracuda model results and the method described above applied to the plant reactor data are compared to several other literature entrainment rate correlations in Table 3. A 5% higher superficial gas velocity was used in the entrainment rate correlations due to the internal blockage inside the reactor around the transport disengagement height (TDH). Evaluating the Barracuda model results in the same manner as the plant data, the average slip factor shown in Figure 5 for each reactor diameter was applied to the pressure drop over height (DP/L) data from the plant to estimate the actual entrainment rate. By using this method, the Barracuda model results include both the actual solids slip and any solids moving down the reactor walls, diplegs, or other structures. Therefore, the Barracuda predicted slip may be reasonably applied to the plant reactor data. Using this same slip factor on the plant DP/L data, the 9-m diameter reactor entrainment at a superficial gas velocity of 0.6 m/s is about 50% of the Barracuda model prediction. The 3.6-m diameter reactor entrainment rate predicted using this method was about 65% of the Barracuda model prediction. A separate independent method of measuring cyclone loading in the plant reactor was reasonably close to these entrainment rate predictions. Ideally, the top two pressure taps would be closer together and closer to the cyclone inlet.

Overall the Barracuda model was as good as or better than most literature correlations. Reasons for the deviation could include the lack of inter-particle forces (clustering) in the Barracuda model vs. the expectation that these are present in the plant reactors, or drag model and bed-expansion differences. Schildermans and Baeyens (3) attempted to correlate entrainment rates Sohio-type Acrylonitrile reactors using a combination of entrainment rate correlations. Using a 3.5-m diameter reactor, they calculated entrainment fluxes of 0.23-0.91 kg/s m^2, which are much lower than those calculated in this study. Possible reasons for the higher estimated fluxes from the plant reactor data compared to Schildermans and Bayeyens or FCC systems include less clumping due to different catalyst systems, higher fines content, and that the real slip factors could be higher than predicted by Barracuda.

Table 3. Entrainment Flux Comparison to Selected Correlations at U_o = 0.6 m/s

	kg /s m^2
3.6-m plant reactor pressure data with 1.83 slip factor applied	11.9
3.6-m Barracuda Model Actual Entrainment	18.6
9-m plant reactor pressure data with 2.44 slip factor applied	7.81
9-m Barracuda Model Actual Entrainment	15.5
PSRI Correlation (4)	2.9
Tasirin and Geldart (4)	1.8
Zenz, et al. Procedure (5)	22.5
Kato, et al. (6)	7.3
Wen and Hashinger (7)	0.4
Geldart et al. (8)	5.9
Merrick and Highley (9)	35.0
Zenz and Weil (10)	1.7
Sciazko (11)	5.6

Interestingly, Abrahamsen and Geldart (12) showed no impact of bed diameter on entrainment rate, and Wen and Chen (13) indicate directionally that the elutriation rate is expected to be higher for larger diameter vessels. Their work contrasts with this study in which both the plant and Barracuda models show decreasing entrainment flux with increasing column diameter. In the case of the plant reactor data, the smaller diameter plant reactor had a higher fines content which may have dominated this difference.

CONCLUSIONS

Barracuda CPFD models showed reasonable fit of pressure vs. height compared to Sohio-type Acrylonitrile reactors of 3.6- and 9-m diameter. Slip factors were calculated over the range of the top two pressure taps of the plant reactors and were used to estimate entrainment rates within 10-50% of the Barracuda model predicted entrainment rates. The Barracuda model slip factor approached 1.55 for the 3.6-m diameter reactor and 1.95 for the 9-m diameter reactor. The Barracuda model fit the 3.6-m diameter reactor data better than the 9-m diameter data. Overall, using the calculated slip factor from the Barracuda models applied to the density above TDH or the Barracuda model directly to estimate entrainment rates from large diameter industrial reactors appears to be a reasonable approach.

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NOTATION

$d_{p\,50}$	=	Mass Mean Particle Diameter
H	=	Total Reactor Height
h	=	Local Reactor Height
ψ	=	Slip Factor
U_o	=	Superficial Gas Velocity
ε_{avg}	=	Average Void Fraction
V_p	=	Particle Velocity
G_s	=	Solids Flux (mass/area-time)
ρ_p	=	Particle Density
g	=	Gravitational Constant
P	=	Pressure
z	=	Vertical Coordinate
dP/dz	=	Pressure Gradient

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