FLUIDIZED-BED REACTOR DESIGN:
Approximate Reasoning and Qualitative Simulation

by

RIZWAN MITHANI

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Approved by :

L. T. Fan
Major Professor

W P Walawender
Co-Major Professor

"My work has always tried to unite the true with the beautiful and when I had to choose one or the other I usually chose the beautiful."

Hermann Weyl
German mathematician

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Chapter 1

INTRODUCTION

When a fluid is passed through a bed of solid particles, or solids in short, they are transformed into a fluid-like state at a sufficiently high velocity (called the minimum fluidization velocity). This phenomenon is termed fluidization. The equipment used for this purpose is called a fluidized bed.

Compared to fixed and moving beds, fluidized beds have a number of advantages, such as convenient handling of solids, low pressure drop, and excellent heat and mass transfer characteristics. Thus, they have been widely employed as chemical reactors. Some of the applications include catalytic reforming, limestone calcination, phthalic anhydride production, Fischer-Tropsch synthesis, coal gasification, and biomass pyrolysis.

Due to the lack of a highly reliable theory of fluidization, the modeling, design and scale-up of fluidized-bed reactors remain an indecisive endeavor. The available knowledge in this domain is often uncertain, approximate, incomplete and qualitative in nature. Recent advances in the developing field of artificial intelligence appear to offer an attractive alternative to express and reason with such information. The objective of this work is to explore the application of artificial intelligence oriented reasoning for modeling, scale-up and design of

fluidized-bed reactors; this is contributory to the ultimate objective of developing an intelligent expert system for fluidized-bed reactor design.

The work is divided into four chapters. Presented below is an overview of each chapter.

Chapter 2 is an exhaustive review and critical analysis of the available contributions to the theory and practice of scaling up fluidized-bed reactors. The significance and limitations of these contributions are compared with one another; moreover, an attempt is made to resolve the contradictions among them. In Chapter 3, various dimensionless groups that need be maintained constant (ideally according to theory) in scaling up fluidized-bed reactors are identified. The relative importance of each of these groups is discussed. Various production rules for scale-up of fluidized-bed reactors are formulated in Chapter 4. The rule set is evaluated using a non-additive evaluative strategy employing linguistic variables. Chapter 5 treats prediction of the bubble size distribution as a significant part of modeling fluidized-bed reactors. A qualitative simulation technique is applied for predicting the bubble-size distribution. The resultant distribution is compared with existing theory and experimental data. Finally, the conclusions and recommendations are discussed in Chapter 6.

Chapter 2

A REVIEW OF EXPERT KNOWLEDGE

Compared to fixed beds and moving beds, fluidized beds have a number of advantages, such as convenient handling of solids, low pressure drop, and excellent heat and mass transfer characteristics. Despite these advantages, fluidized-bed processing devices have often failed to perform to their expectations. The cause of this is the extremely complex nature of the fluidization phenomenon; a highly reliable theory of fluidization capable of predicting fluidization behavior in large beds is lacking. Thus, most commercial fluidized-bed reactors are designed by scaling up laboratory-scale reactors. This necessitates a knowledge of scaling relationships among the reactors (see, e.g., Broadhurst and Becker,1973; Fitzgerald et al., 1984; Glicksman, 1984). The objectives of this chapter are to review and critically analyze the available expert knowledge on such scaling relationships.

CRITICAL ANALYSIS

During the course of reviewing the available literature in fluidized-bed reactor scale-up, four different similarities have been identified; these include (a)hydrodynamic similarity, (b)chemical similarity, (c)geometric similarity, and (d)particle similarity.

Therefore, the critical review is divided into four sections based on the various kinds of similarities.

Hydrodynamic Similarity

Literature abounds with various parameters to characterize the hydrodynamics in a fluidized bed. The work by Matsen (1970,1985) and Glicksman (1984) in this area appear to be of particular significance.

According to Matsen (1970), the following hydrodynamic parameters affect reactor performance;

(i) Effective space time: It is the product of the bubble residence time and bubble gas fraction instantaneously associated with the emulsion phase. To hold this constant requires keeping the ratio

$$\frac{H_{mf}}{(U - U_{mf})\sqrt{D}}$$

fixed (Matsen, 1970). This is essential for slow reactions.

(ii) Fraction of bubble gas exchanged: To keep constant the fraction of bubble gas exchanged with the emulsion phase in both small and large scale beds, the ratio

$$\frac{H_{mf}}{(U - U_{mf})D}$$

should be held constant if possible (Matsen, 1970). This is important for fast reactions.

(iii) Bubble residence time: The amount of time a bubble resides in the fluidized bed is the ratio of bed height to bubble velocity. This requires that

$$\frac{H_{mf}}{\sqrt{D}}$$

be maintained constant. The bubble residence time is particularly important for non-catalytic reactions.

(iv) Relative bed expansion: For entrance effects to have the same relative influence at different scales, the ratio H/H_{mf} need be maintained constant. This is achieved by keeping

$$\frac{(U - U_{mf})}{\sqrt{D}}$$

invariant (Matsen, 1970). It may be noted that this is required even by the condition for geometrically similar bubble coalescence (Horio et al., 1986).

(v) Height-to-diameter ratio: H_{mf}/D should be kept constant for minimizing entrance effects in beds of different sizes.

Utilizing the scale-up criteria presented in the preceding paragraph has two disadvantages. Firstly, these scale-up ratios are inherently conflicting, and it is difficult to maintain more than two of them constant simultaneously. Secondly, the ratios are not dimensionless, and attempting to maintain them invariant is not a sound engineering practice.

There has been rather extensive effort to identify the dimensionless groups that should be maintained constant to ensure hydrodynamic similarity. The Reynolds number, Froude number, solid-to-fluid density ratio, and height-to-diameter ratio are the four dimensionless groups identified by Romero and Johanson (1962), Broadhurst and Becker (1973), and Fitzgerald et al.(1984). These researchers have experimentally verified the scaling laws governed by these dimensionless groups.

A systematic attempt to identify the significant dimensionless groups has been made by Glicksman (1984). The governing equations of motion and continuity are written for both the fluid and particles. These equations are then non-dimensionalized. Moreover, the boundary conditions are written in terms of dimensionless length scales. His study has resulted in the identification of the following controlling dimensionless groups;

$$\frac{\beta d_p}{\rho_s U^2}, \frac{g d_p}{U^2}, \frac{H}{d_p}, \frac{D}{d_p} \text{ and } \frac{\rho_f}{\rho_s}$$

where the drag coefficient β is related to other bed properties through the Ergun equation for pressure drop through a packed bed

$$\frac{\beta d_p}{\rho_s U} = \frac{-\Delta P}{H} = \frac{150(1 - \epsilon_{mf})^2 \mu_f U}{\epsilon_{mf}^3 (\phi_s d_p)^2} + \frac{1.75(1 - \epsilon_{mf}) \rho_f U^2}{\epsilon_{mf}^3 \phi_s d_p} \quad (2\text{-}1)$$

After non-dimensionalization, it is simplified by dropping the first term in the right-hand side, i.e., viscous

contribution, when the Reynolds number based on the fluid density is greater than 400; when it is less than 4, the second term on the right-hand side, i.e., the inertial contribution, may be neglected. The former case represents the inertial limit, for which Glicksman (1984) has identified the governing parameters to be;

$$\frac{gd_p}{U^2}, \frac{H}{d_p}, \frac{D}{d_p}, \frac{\rho_f}{\rho_s} \text{ and } \phi_s$$

In the latter case, corresponding to the viscous limit, he has identified the governing parameters to be;

$$\frac{gd_p}{U^2}, \frac{H}{d_p}, \frac{D}{d_p}, \frac{\rho_s U d_p}{\mu_f} \text{ and } \phi_s$$

All these parameters except one are common to both limits. For the intermediate region, all the parameters need be maintained constant.

Though the approach of Glicksman (1984) seems attractive, it suffers from the following deficiencies;

(i) The inertial and viscous limits cannot be clearly defined.

(ii) It involves keeping a large number of parameters invariant merely to ensure the hydrodynamic similarity.

(iii) The smaller the scale of a bed, the smaller the size of particles in it. This implies that the powder classification of the particles might change.

(iv) It does not take into account the fact that, in general, small beds tend to slug, while large beds do not.

Zhang and Yang (1987) have published a work similar to that of Glicksman (1984) on scaling up cold, small-scale, laboratory beds to hot, large-scale, commercial beds. According to them we may resort to two length scales, D and d_p, in non-dimensionalizing the governing equations. This requires that the ratio, D/d_p, be kept constant in scaling up, thereby necessitating that beds of different sizes contain particles of different sizes. However, Zhang and Yang (1987) have noted that the gas flow and solids mixing are mainly controlled by the bubbling phenomenon in a bubbling fluidized bed. Widely employed correlations for estimating the bubble velocity and bubble diameter do not involve the particle diameter as a parameter; this implies that it is insignificant in bubbling fluidization, and therefore, D/d_p need not be held constant.

The significance of slugging in scaling up fluidized-bed reactors deserves due attention; otherwise, the hydrodynamic similarity obtained through maintaining the dimensionless groups invariant may be misleading. Numerous pilot-scale, fluidized-bed reactors operate in the slug flow regime, where the bubble diameter approaches the column diameter, and the gas flows upwards in the form of a slug (see Fig. 2-1). Commercial-scale, fluidized-bed reactors, being larger in diameter, tend to exhibit bubbling behavior, as the wall effect is negligible in them. Thus, it is essential to determine the maximum column diameter for which slugging

will occur. Fluidized beds of approximately 0.6 m (25 inches) or more in diameter have exhibited slug flow (Matsen, 1970). Theoretically, the maximum column diameter in which slugging can occur is four times the maximum stable bubble size (Matsen, 1970). The reason for this is that the velocity of a bubble is twice that of a slug of the same diameter. The bubble velocity and the slug velocity are proportional to the square root of the bubble diameter and the slug diameter, respectively. Stewart and Davidson (1967) have derived the following criterion for onset of slugging;

$$U_{ms} = U_{mf} + 0.07\sqrt{gD} \qquad (2\text{-}2)$$

Chemical Similarity

Some of the applications of fluidized beds as chemical reactors include catalytic reforming, acrylonitrile production, Fischer-Tropsch synthesis, thermal cracking, and coal gasification (see, e.g., Kunii and Levenspiel, 1977). To be able to predict the conversion in a commercial-scale, fluidized-bed reactor is essential to its design.

One of the early attempts at modeling has resulted in the development of the bubbling bed model (Kunii and Levenspiel, 1977). This model, however, suffers from the assumption of a constant bubble size throughout the bed. Kato and Wen (1969) have proposed the bubble assemblage model; in this model, the bed is divided into compartments,

each with a constant bubble size. The bubble assemblage model is convenient for computer simulations. Another significant contribution to fluidized-bed reactor modeling is the countercurrent backmixing model (Fryer and Potter, 1972); it takes into account the observed flow reversal at the critical superficial velocity.

Although substantial effort has been made in developing models, numerous difficulties encountered in scaling up fluidized-bed reactors are yet to be satisfactorily resolved. The scale-up and design of fluidized-bed reactors remain an indecisive endeavor due to the unreliability and dubitable predictive power of the models.

Van Swaaij and Zuiderwig (1973) have proposed the following empirical equation for the height of a cross-flow unit;

$$H_X = \frac{H}{N_X} = \left[1.8 - \frac{1.06}{D^{1/4}}\right]\left[3.5 - \frac{2.5}{H^{1/4}}\right] \qquad (2\text{-}3)$$

where D and H are in meters; the number of cross-flow units, N_X, is defined as

$$N_X = \frac{H\alpha}{U} \qquad (2\text{-}4)$$

Based on this correlation, Matsen (1985) has proposed a method to scale-up fluidized-bed reactors. His algorithmic method allows prediction of the conversion in a commercial-scale, fluidized-bed reactor, provided that the kinetic data obtained with a laboratory-scale reactor are available, and

the proposed capacity for commercial operation is specified. The methodology is attractive as it takes into account the fact that a smaller bed tends to slug while a larger bed does not. Nevertheless, it should be remembered that the correlation of Van Swaaij and Zuiderwig has been proposed and verified only for relatively slow reactions and Group A particles (classification of particles is discussed under the section "Particle Similarity" in detail, later).

The model of Orcutt et al. (1962) has been systematically analyzed by Grace (1980). This model assumes that the gas is in plug flow in the bubble phase and the emulsion phase is perfectly mixed. Furthermore, the bubble phase is assumed to be free of solids. The governing equations of the model have been solved by Grace (1980) for zero-order irreversible, half-order irreversible, first-order irreversible, second-order irreversible, first-order reversible and consecutive first-order reactions. The resultant solutions have been presented in terms of the dimensionless outlet concentration, C_{out}/C_{in}. This concentration is a function of the following three parameters in all cases;

(i) Dimensionless rate constant

$$k_n' = \frac{k_n H_{mf}(1 - \epsilon_{mf})(C_{in})^{n-1}}{U} \qquad (2\text{-}5)$$

(ii) Dimensionless interphase mass transfer group

$$X = \frac{k_{be} a \epsilon_b H}{(U - U_{mf})} \qquad (2\text{-}6)$$

(iii) Fraction of gas flowing through bubble phase

$$f_b = \frac{(U - U_{mf})}{U} \qquad (2\text{-}7)$$

It is worth noting that the model underestimates the conversion for fast reactions, since it assumes an absence of solids in the bubble phase.

By resorting to an approach similar to that of Grace (1980), Van Swaaij (1985) has identified the following three dimensionless groups which need be maintained invariant in scale-up;

(i) Number of reaction units

$$N_R = \frac{k_r(1 - \epsilon_b)H}{U} \qquad (2\text{-}8)$$

(ii) Effective dimensionless mass transfer rate

$$N_X = \frac{\alpha H}{U} \qquad (2\text{-}9)$$

(iii) Effective dimensionless mixing rate in the gas phase

$$N_D = \frac{UH}{f_e E_G} \qquad (2\text{-}10)$$

Close observation of these groups indicates that the dimensionless rate constant defined by Grace and the number of reaction units defined by Van Swaaij represent the same

notion. Moreover, the dimensionless mass transfer groups defined by these two authors embody the same concept. The effective dimensionless mixing rate involves the fraction of the gas flowing through the emulsion phase, f_e, in the denominator. Note that

$$f_e = 1 - f_b \qquad (2\text{-}11)$$

Thus, maintaining f_b invariant as proposed by Grace implies keeping f_e constant. In essence, therefore, Van Swaaij has included a dimensionless group UH/E_G to be maintained constant in addition to those of Grace for ensuring similarity in the mixing pattern in beds of different scales.

Figure 2-2 illustrates the effect of the number of mixing units, N_D, the number of reaction units, N_R, and the number of mass transfer units, N_X, on the conversion in a fluidized-bed reactor.

Geometric Similarity

Theoretically, to achieve successful scale-up, complete geometrical similarity should exist between the small-scale and large-scale beds. However, we can never really achieve complete geometrical similarity (see, e.g., Astarita, 1985). In principle, it is possible to have the same height-to-diameter ratio for the two different scales. Nevertheless, it is impossible, for instance, to scale-up completely the geometry of the catalyst particles used.

A similarity rule has been proposed by Horio et al. (1986) for scale-up of bubbling fluidized beds. This rule is based on the governing equations for dynamics of bubble and interstitial gas flows. Through non-dimensionalization of these equations, they have proposed the following two rules;

(A) Condition for geometrically similar bubble coalescence:

$$U - U_{mf} = \sqrt{m}\ (U - U_{mf})_p \qquad (2\text{-}12)$$

(B) Condition for geometrically similar bubble splitting and interstitial gas flow:

$$U_{mf} = \sqrt{m}\ (U_{mf})_p \qquad (2\text{-}13)$$

The subscript, p, in the equations (2-12) and (2-13) refers to conditions in the pilot-scale bed, and m represents the scale-up factor which is explicit in Fig. 2-3. The validity of the similarity rules, equations (2-12) and (2-13), has been tested only for Group B particles. We know that when using particles belonging to Group B, which have the same density in both large and small scale beds,

$$U_{mf} \propto d_p^2 \qquad (2\text{-}14)$$

Thus, the rule implicitly involves the change in the particle size by a factor $m^{1/4}$. This can lead to the change in powder characteristics between the two different scales. For instance, for a scale-up factor m of 20, its fourth root would be 2.11. Hence, we would have to use in the larger-scale bed, particles more than twice the size of particles

in the smaller-scale bed. These would probably not belong to the same powder group.

The rules of Horio et al. (1986) take into account slugging behavior in beds. The behavior of slugs and the onset condition of slugging, as given by Stewart and Davidson (1967), are consistent with this similarity rule. The slug velocity is given as (Stewart and Davidson, 1967)

$$\frac{U_s}{\sqrt{gD}} = \frac{(U - U_{mf})}{\sqrt{gD}} + 0.35 \qquad (2\text{-}15)$$

The right-hand side of this expression would remain constant with scaling. Thus, to maintain the left-hand side constant would imply

$$U_s = \sqrt{m}\, U_s^p \qquad (2\text{-}16a)$$

and

$$U_s - U_{mf} = \sqrt{m}\, (U_s - U_{mf})^p \qquad (2\text{-}16b)$$

For onset of slugging (Stewart and Davidson, 1967),

$$\frac{(U_{ms} - U_{mf})}{\sqrt{gD}} = 0.007 \qquad (2\text{-}17)$$

Note that the left-hand side of this equation would remain constant for all values of m. Thus, if the laboratory-scale bed exhibits slugging behavior, the commercial-scale bed would also exhibit such behavior.

Particle Similarity

Maintaining particle or powder similarity is essential for scaling up a fluidized-bed reactor. For optimum

performance of such a reactor, effective solids-fluid contacting and solids circulation are necessary. In general, the quality of fluidization is dependent on the particle characteristics.

The most widely used powder classification scheme is the one developed by Geldart (1973; 1980). It describes the fluidization behavior of solid particles. A convenient classification has been suggested in which the various powders are arranged into four groups, viz. C,A,B and D. Figure 2-4, which is a plot of $(\rho_s - \rho_f)$ against d_p, under constant pressure and temperature, depicts the classification.

Cohesive Group C powders or particles are characterized by their very small sizes ($d_p < 30\mu m$); they are extremely difficult to fluidize. This can be attributed to their strong electrostatic charges and to their wet and sticky particle surfaces. Talc is an example of the Group C powder.

The sizes of Group A particles are relatively small ($d_p = 30 - 150\mu m$) and their densities relatively low ($\rho_s < 1500 kg/m^3$). The minimum bubbling velocity, U_{mb}, of these particles is always greater than the minimum fluidization velocity, U_{mf}. Most commercial catalysts used in fluidized beds belong to this group.

Typically, Group B particles are materials with larger particle sizes ($d_p = 150 - 500\mu m$) and higher densities ($\rho_s =$

1500 - 4000kg/m^3). Here, the minimum bubbling velocity, U_{mb}, is approximately equal to the minimum fluidizing velocity, U_{mf}. Glass beads are an example of Group B particles.

Group D comprises very large and/or dense particles. These particles can be made to spout even in deep beds. Crushed limestone and coffee beans are examples of this particle type.

The boundary criteria for the above groups are as follows;

(i) Group C/A boundary

It is shown as band AC in Fig.2-4. According to Molerus (1982), a powder belongs to Group C if

$$\frac{(\rho_s-\rho_f)d_p^3 g}{F_H} < 10^{-3} \qquad (2\text{-}18)$$

Here F_H represents the adhesive force transmitted in a single contact between two particles.

(ii) Group A/B boundary

A powder will be in Group A or C if

$$\rho_s^{0.934} d_p^{0.8} < 1 \qquad (2\text{-}19)$$

Equation (19) is shown as line AB in Fig.2-4.

(iii) Group B/D boundary

Baeyens and Geldart (1973) have proposed the numerical criterion that if

$$(\rho_s-\rho_f)d_p^{1.24} > 0.23, \qquad (2\text{-}20)$$

then the powder is spoutable and belongs to Group D. Equation (20) is plotted as line CD in Fig.2-4.

According to Saxena and Ganzha (1984), the Group D particles of Geldart (1973;1980) regarded as large particles can be small particles from a heat transfer point of view. It is, therefore, necessary to consider simultaneously hydrodynamics and heat transfer behavior of these particles in scaling up fluidized beds. The latter is characterized by the Nusselt number, whereas the former is characterized by the Reynolds number. Both these dimensionless groups are uniquely dependent on the Archimedes number, Ar. Thus, Saxena and Ganzha base their powder classification on this dimensionless group; it is defined as

$$Ar = \frac{d_p^3 g \rho_f (\rho_s - \rho_f)}{\mu_f^2} \qquad (2\text{-}21)$$

Consequently, the powders may be classified into four groups as

Group I : $1600 < Ar < 21700$

Group IIA : $21700 < Ar < 1.3 \times 10^5$

Group IIB : $1.3 \times 10^5 < Ar < 1.6 \times 10^6$

Group III : $Ar > 1.6 \times 10^6$

These particle groups are all within the domain of Geldart's Group D particles. Essentially, the classification scheme of Saxena and Ganzha is intended for large particle systems. Particles belonging to Geldart's other three groups are not represented in the scheme of Saxena and Ganzha, as they

would be small particles from the viewpoints of both hydrodynamics and heat transfer.

In scaling up, caution should be exercised to ensure that particles fall into the same category for different scales so that the quality and nature of fluidization remain essentially invariant.

CONCLUSIONS

Due to the lack of a highly reliable fluidization theory, most of the commercial fluidized-bed reactors are designed by scaling up laboratory-scale reactors. This necessitates a knowledge of scaling relationships among the reactors.

During the course of reviewing the available literature in fluidized-bed reactor scale-up, four different similarities have been identified; these include: (a) hydrodynamic similarity, (b) chemical similarity, (c) geometric similarity, and (d) particle similarity.

Numerous researchers have identified a variety of dimensionless groups that need be maintained constant to ensure hydrodynamic similarity. The important groups include the Reynolds number, Froude number, solid-to-fluid density ratio, and height to diameter ratio.

Even with substantial effort at modeling, the design and scale-up of fluidized-bed reactors remain an indecisive endeavor. The four important dimensionless groups

identified to ensure chemical similarity include the number of reaction units, number of mass transfer units, number of mixing units, and bubble phase gas fraction.

We can never achieve complete geometric similarity. Nevertheless, two similarity rules, based on geometrically similar bubble coalescence, and geometrically similar bubble splitting and interstitial gas flows, are available. The validity of these rules has been tested only for Group B particles. The rules coincidently take the slugging behavior into account.

Ensuring particle or powder similarity based on hydrodynamics leads to a similar quality of fluidization for different scales. The classification of particles into Geldart's Groups C,A,B and D is widely used. A classification scheme based on the heat transfer behavior, is also available for large particles.

NOTATION

a	=	interficial bubble area per unit bubble volume	$[m^2/m^3]$
Ar	=	Archimedes number	[-]
C_{in}	=	inlet concentration	$[Kmol/m^3]$
C_{out}	=	outlet concentration	$[Kmol/m^3]$
d_o	=	size of distributor hole	[m]
d_p	=	particle diameter (average)	[m]
D	=	bed diameter	[m]

D_b	=	bubble diameter	[m]
E_G	=	axial mixing coefficient of the emulsion phase	[m^2/s]
f_b	=	fraction of gas flowing through the bubble phase	[-]
f_e	=	fraction of gas flowing through the emulsion phase	[-]
F_H	=	adhesive force transmitted between two particles	[-]
g	=	acceleration due to gravity	[m/s^2]
H	=	bed height	[m]
H_{mf}	=	height at minimum fluidization	[m]
H_X	=	height of a cross-flow unit	[m]
k_{be}	=	bubble to emulsion phase mass transfer coefficient	[m/s]
k_n	=	reaction rate constant, for the n-th order reaction	[-]
k'_n	=	dimensionless rate constant	[-]
k_r	=	reaction rate constant based on the emulsion phase volume	[s^{-1}]
m	=	scale-up factor	[-]
n	=	order of reaction	[-]
N_D	=	number of mixing units	[-]
N_R	=	number of reaction units	[-]
N_X	=	number of mass transfer units / cross-flow units	[-]
p	=	superscript for pilot-scale bed properties	[-]
p_n	=	distributor pitch	[m]
U	=	superficial fluid velocity	[m/s]
U_{mf}	=	minimum fluidization velocity	[m/s]

U_{ms}	=	minimum superficial velocity required for slugging	[m/s]
U_s	=	slug velocity	[m/s]
X	=	dimensionless interphase mass transfer group	[-]
α	=	mass exchange coefficient based on the bed volume	[s^{-1}]
β	=	coefficient of drag force	[$kg/m^3/s$]
Δp	=	pressure drop	[N/m^2]
ϵ_b	=	fraction of the bed volume occupied by bubbles	[-]
ϵ_{mf}	=	voidage at minimum fluidization	[-]
μ_f	=	viscosity of the fluid	[kg/m/s]
ρ_f	=	density of the fluid	[kg/m^3]
ρ_s	=	density of the solid	[kg/m^3]
ϕ_s	=	sphericity	[-]

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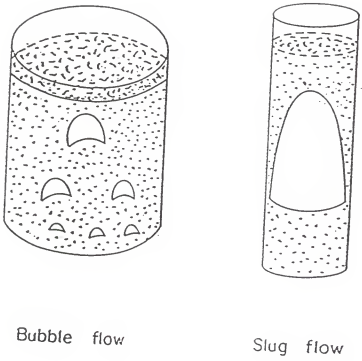

Fig. 2-1. Bubble and slug flow in fluidized beds.

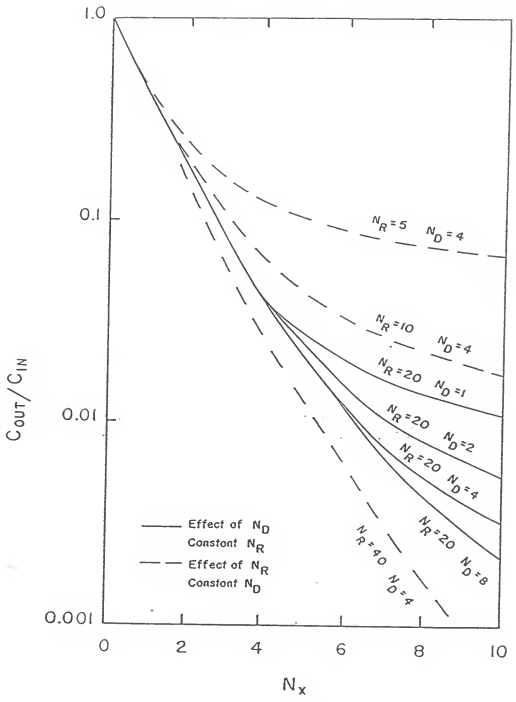

Fig. 2-2. Effect of N_X, N_D and N_R on conversion (Matsen, 1985)

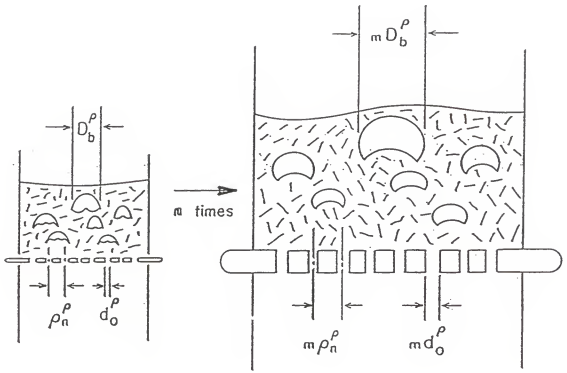

Fig. 2-3. Geometrically similar fluidized beds.

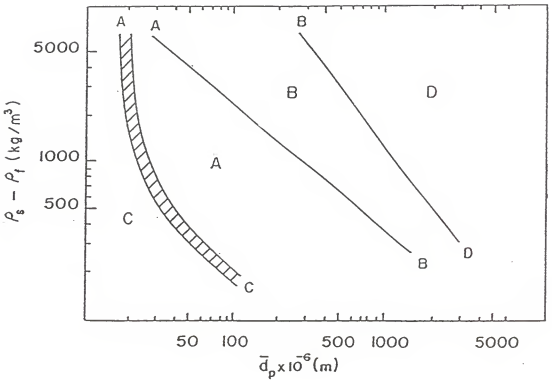

Fig. 2-4. Geldart's powder classification.

Chapter 3

IDENTIFICATION OF DIMENSIONLESS GROUPS

The *Similarity Principle* involves establishing relationships between the corresponding governing parameters in fluidized-bed reactors of different sizes. Such relationships may be instituted by maintaining the dimensionless groups describing the fluidization phenomenon invariant. From the exhaustive review of available information and knowledge presented in Chapter 2, the following dimensionless groups have been identified;

(a) Reynolds number, Re

(b) Froude number, Fr

(c) Archimedes number, Ar

(d) Linear dimension ratio, λ

(e) Density ratio, ω

(f) Bubble phase gas fraction, f_b

(g) Number of reaction units, N_R

(h) Number of mass transfer units, N_X

(i) Number of mixing units, N_D

CRITICAL ANALYSIS

The relative significance of the identified dimensionless groups for various situations is discussed below.

Reynolds Number, Re

Physically, the Reynolds number is the ratio of inertial forces to viscous forces. While it is defined variously based on different variables or parameters, in general,

$$Re = \frac{(\text{characteristic length})(\text{velocity})(\text{density})}{(\text{viscosity})}$$

The viscosity is invariably taken to be that of the fluid or fluidizing medium. Most researchers use the particle diameter, d_p, as the characteristic length. Nevertheless, Zhang and Yang (1987) have used the bed diameter D, instead. The former choice is more rational than the latter one, as the flow around particles is characterized by the particle diameter, especially in relatively large beds.

Some authors (e.g., Romero and Johanson ,1962) base the Reynolds number on the minimum fluidization velocity, U_{mf}, while most others (e.g., Broadhurst and Becker, 1973; Fitzgerald et al., 1984; Glicksman, 1984; Saxena and Ganzha, 1984; Zhang and Yang, 1987) base it on the superficial fluid velocity, U.

The choice of density also varies. Romero and Johanson (1962) have proposed the use of ρ_f for liquid fluidization, but ρ_s for gas fluidization. Glicksman (1984) has used ρ_s in Re_s as the dimensionless group to be kept constant, but has used ρ_f in Re_f to specify the inertial and viscous limits. Most others (Broadhurst and Becker, 1973;

Fitzgerald et al., 1984; Saxena and Ganzha, 1984) employ ρ_s. Thus, in determining the significance of the Reynolds number, it is essential to know its actual basis. While numerous researchers (e.g., Saxena and Ganzha, 1984; Glicksman, 1984) have specified ranges of the Reynolds number, they should be used with extreme caution because their bases may be different.

According to Glicksman (1984), it is necessary to maintain Re_s constant in the viscous limit, but not in the inertial limit. Re_s is also an essential parameter at relatively high pressures, and for particles of relatively small sizes. Since most of the correlations for heat and mass transfer involve the Reynolds number, this dimensionless group need be maintained constant when these transfer processes play prominent roles in the reactor to be scaled up.

It is not always essential to maintain the Reynolds number constant. In most cases, it is sufficient to maintain it within a certain range between the two scales; it relaxes a constraint involved in the scale-up of fluidized-bed reactors. The ranges are specified by Glicksman's viscous and inertial limits. Also, these need be superimposed by the ranges proposed by Saxena and Ganzha (1984) such that the powder classification remains the same (see Table 3-1).

Froude Number, Fr

The Froude number can be interpreted as the ratio of inertial forces to the gravity forces exerted on particles, i.e.,

$$Fr = \frac{(\text{velocity})^2}{(\text{acceleration due to gravity})(\text{linear dimension})}$$

Wilhelm and Kwauk (1948) appear to be the first to use the Froude number as a criterion to distinguish between particulate and aggregative fluidization. According to them,

$Fr < 0.13$ – particulate

$Fr > 1.3$ – aggregative

while Brown (1951) classifies it as

$Fr < 1$ - particulate

$Fr > 1$ - aggregative

In both cases, the Froude number is based on the minimum fluidization velocity and particle diameter.

Fitzgerald et al. (1984) define the number as Hg/U^2, while Glicksman (1984) defines it as gd_p/U^2 (note that these definitions are inverse of the above definition; this is not uncommon in fluidized bed literature). The latter definition appears to be a more appropriate choice, as flow is characterized around the particle, thereby rendering d_p significant. Moreover, U should be used rather than U_{mf}, as U represents the operating velocity of the fluid in the bed. These authors define the Froude number with the square of the velocity in the denominator. To maintain consistency,

it is suggested that the square of the velocity be in the numerator.

Fitzgerald et al. (1984), Zhang and Yang (1987), and Glicksman (1984) have all identified the Froude number as an important parameter to be maintained constant for the entire range of the Reynolds number. Since this may not always be possible, caution should be exercised to ensure that this group is maintained within the three ranges implicitly specified by Wilhelm and Kwauk (1948) to maintain the bed within a certain fluidization regime.

Archimedes Number, Ar

The Archimedes number signifies the ratio of the gravitational forces to the viscous forces exerted on the fluidized particles. By definition,

$$Ar = \frac{d_p^3 g \rho_f (\rho_s - \rho_f)}{\mu_f^2} \qquad (3\text{-}1)$$

As seen in chapter 2, the Nusselt number characterizing the rate of heat transfer is related to the Archimedes number. Therefore, according to the analysis of Saxena and Ganzha (1984), this dimensionless group must be maintained in the ranges discussed earlier such that the powder classification does not change. This would gain significance if the particles are large (Geldart's Group D) and heat transfer is salient to the situation at hand.

A modified form of the Archimedes number is

$$Ar = \frac{d_p^3 g \rho_s^2}{\mu_f^2} = \frac{\left[\frac{d_p U \rho_s}{\mu_f}\right]^2}{\left[\frac{U^2}{g d_p}\right]} \qquad (3\text{-}2)$$

which is essentially the ratio of square of the Reynolds number to the Froude number. According to Glicksman (1984), it is essential to maintain this dimensionless group constant in the viscous limit, i.e., $Re_f < 4$.

Linear Dimension Ratio, λ

This ratio is a direct consequence of the geometric similarity criterion. It has been variously defined.

Matsen(1970;1985) proposes keeping H_{mf}/D or H/D constant while scaling. This permits us to maintain the entrance effects constant in beds of different sizes. Furthermore,this criterion is consequential for

(i) low superficial fluid velocity,

(ii) a shallow fluidized bed, and

(iii) a small diameter bed.

Fitzgerald et al. (1984) have proposed λ to be H/d_p. Similarly, the analysis by Glicksman (1984) requires that both H/d_p and D/d_p be maintained constant in beds of different sizes for all ranges of the Reynolds number. Romero and Johanson (1962) have contended that D/d_p and H_{mf}/D be kept invariant in scaling. Obviously, Glicksman's criterion implies that the third ratio H/D be kept constant.

Similarly requiring the third ratio H_{mf}/d_p to be invariant is implicit in Romero and Johanson's contention. Keeping the ratio H/D fixed is necessary to ensure geometric similarity of beds of different sizes (Horio et al., 1986).

H/D is a more appropriate choice compared to H_{mf}/D, as the former represents the operating condition, which determines the performance of the concerned process. In most cases it is impractical to maintain D/d_p invariant; this is because changing the particle diameter with changing scales may imply altering the powder classification and ,hence, the quality of fluidization. Moreover, it may not always be possible to obtain particles, e.g., grain, in different sizes. As noted earlier, the ratio D/d_p need not be held constant for bubbling fluidization (Zhang and Yang, 1987).

Density Ratio, ω

ω is widely accepted as the ratio of solid to fluid densities or that of fluid to solid densities,i.e.,

$$\omega = \frac{\rho_s}{\rho_f}$$

or

$$\omega = \frac{\rho_f}{\rho_s}$$

Analysis of Glicksman (1984) indicates that ω is a significant criterion to be kept invariant in the inertial limit, i.e., $Re_f > 400$. Its importance increases with an increase in pressure and a decrease in particle size.

Some researchers, e.g., Romero and Johanson (1962), have proposed the use of $(\rho_s - \rho_f)$ instead of ρ_s when the fluid is a liquid. This implies that the ratio $(\rho_s - \rho_f)/\rho_f$ be employed for liquid fluidization and the ratio ρ_s/ρ_f for gas fluidization. Nevertheless, it is worth noting that the latter ratio is automatically taken into account by the former ratio, and thus the use of the former should be generally preferred.

Bubble Phase Gas Fraction, f_b

f_b is the fraction of gas flowing into the bubble phase. Conversion in a fluidized-bed reactor is a function of f_b (Grace, 1980; Matsen, 1985). This has been derived by Grace (1980) for different-order reactions using the model of Orcutt et al. (1962). Thus, f_b need be kept constant in scaling up fluidized-bed reactors. According to the two-phase theory of fluidization,

$$f_b = \frac{(U - U_{mf})}{U} \tag{3-3}$$

as all gas after minimum fluidization is assumed to flow through the bubble phase. For higher order reactions, prediction of conversion is more sensitive to f_b; therefore, f_b gains a greater significance, as the reaction order increases.

The effect of f_b on conversion is negligible for $U >> U_{mf}$. Thus, maintaining f_b invariant may not be as meaningful

for such a situation. Again, the conversion is virtually independent of f_b for slow reactions (Grace, 1980), thereby rendering it an insignificant criterion for such reactions.

Number of Reaction Units, N_R

N_R may be defined as the ratio of the bed height to the height of a reaction unit. It relates the amount of solids present to the flow rate and kinetic rate constant.

As noted earlier, N_R has been based on different variables, but in general, it may be represented as

$$N_R = \frac{kH}{U} \tag{3-4}$$

which is an insignificant criterion when

(i) $N_R >> N_X$, and

(ii) N_R is very large.

For relatively slow reactions, the outlet concentration and hence the conversion are controlled by N_R, thereby rendering it an important criterion for such reactions.

In chapter 2, a plot of the effect of N_R, N_x and N_D has been shown in Fig. 2-2. Analysis of this plot leads to interesting conclusions about the significance of N_R. It is of no consequence when N_X is less than 1. For N_X greater than 8, the resultant conversion is always less than 10%, independent of the value of N_R, possibly rendering it unimportant for such a situation.

Number Of Mass Transfer Units, N_X

N_X may be defined as the ratio of the bed height to the height of a mass transfer unit (or cross-flow unit). Physically, it represents the number of times bubble gas is exchanged with emulsion gas (i.e., gas which flows through the emulsion phase) during the bubble rise through the fluidized bed.

Though N_X has been defined based on various parameters, in essence, it may be represented as

$$N_X = \frac{\alpha H}{U} \qquad (3\text{-}5)$$

N_X is an inconsequential criterion when

(i) $N_X >> N_R$, and

(ii) N_X is very large.

N_X is an important criterion when

(i) N_R is very large, and

(ii) the reaction is very rapid.

Again, Fig. 2-2 demonstrates that N_X is a relatively unimportant criterion to be maintained invariant when its value is less than 1. For N_X greater than 8, the conversion obtained is always less than 10%, independent of the value of N_X, possibly rendering it insignificant in such a situation.

Number Of Mixing Units, N_D

N_D may be defined as the ratio of the bed height to the height of a mixing unit (or dispersion unit). It relates the amount of solids present to the superficial velocity and the axial mixing coefficient in the emulsion phase. N_D may be conveniently represented as

$$N_D = \frac{UH}{f_e E_G} \tag{10}$$

We may draw some inferences about the significance of N_D from Fig. 2-2:

(i) It is insignificant when N_X is less than 1.

(ii) It is possibly unimportant when N_X is greater than 8, as under such a situation the conversion obtained is always less than 10%, independent of the value of N_D in such situations.

(iii) It is insignificant when N_R is very large.

CONCLUSIONS

The similarity principle of scale-up involves establishing relationships between fluidized beds of different sizes, by maintaining governing dimensionless groups constant. Fluidization is an extremely complex phenomenon; this has led to the identification of a large number of governing dimensionless groups. These include the Reynolds number, Froude number, Archimedes number, linear dimension ratio, density ratio, bubble phase gas

fraction, Number or reaction units, Number of mass transfer units, and Number of mixing units. In reality, it is impossible to maintain all of them invariant. This is due to the fact that many of the groups may naturally be in conflict with each other. Moreover, additional constraints may be imposed due to the nature of the process as well as pragmatic points of views. Nevertheless, it is possible to weigh the effects of different criteria on the various groups to determine their importance to a particular or specific case.

NOTATION

Ar	=	Archimedes number	[-]
d_p	=	particle diameter	[m]
D	=	bed diameter	[m]
E_G	=	axial mixing coefficient of the emulsion phase	[m^2/s]
f_b	=	fraction of gas flowing through the bubble phase	[-]
f_e	=	fraction of gas flowing through the emulsion phase	[-]
Fr	=	Froude number	[-]
g	=	acceleration due to gravity	[m/s^2]
H	=	bed height	[m]
H_{mf}	=	height at minimum fluidization	[m]
N_D	=	number of mixing units	[-]
N_R	=	number of reaction units	[-]

N_X	=	number of mass transfer units / cross-flow units	[-]
Re	=	Reynolds number	[-]
U	=	superficial fluid velocity	[m/s]
U_{mf}	=	minimum fluidization velocity	[m/s]
α	=	mass exchange coefficient based on the bed volume	[s^{-1}]
λ	=	linear dimension ratio	[-]
μ_f	=	viscosity of the fluid	[kg/m/s]
ρ_f	=	density of the fluid	[kg/m^3]
ρ_s	=	density of the solid	[kg/m^3]
ω	=	density ratio	[-]

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Table 3-1. Fluidization Characteristics Based on the Reynolds Number.

Reynolds # range	characteristics
$0 < Re < 1$	laminar flow(Group I), viscous region
$1 < Re < 4$	extended laminar flow(Group I), viscous region
$4 < Re < 10$	extended laminar flow(Group I), intermediate region
$10 < Re < 40$	transitional flow(Group IIA), intermediate region
$40 < Re < 200$	transitional flow(Group IIB), intermediate region
$200 < Re < 400$	turbulent flow(Group III), intermediate region
$400 < Re < \infty$	turbulent flow(Group III), inertial region

Chapter 4

APPROXIMATE REASONING FOR SCALE-UP RULES

The process of attaining a successful design of a large-scale system based on the empirical information obtained experimentally with a small-scale system and theoretical analysis is termed "scale-up." The "Principle of Similarity" is a cornerstone of equipment scale-up in the chemical process industry. This principle involves setting up relationships between different sized equipment. Such relationships may be instituted by maintaining the dimensionless groups, characterizing the phenomena of the process, invariant (see, e.g., Trambouze, 1977; Astarita, 1985).

For complex phenomena, for instance fluidization, it is nearly impossible to maintain all the governing dimensionless groups constant. However, it should be possible to weigh the effects of various criteria to determine the importance of maintaining a dimensionless group constant in a particular or specific case (see, e.g., Bisio, 1985). Thus, in scale-up, it is necessary to employ a trade-off technique in deciding which specific dimensionless groups are to be maintained invariant.

The scale-up of a process equipment involving complex physico-chemical phenomena, resorting to the principle of similarity, gives rise to a multi-criteria decision making problem. The production rule formalism appears to be

particularly applicable to such a problem. Moreover, it is convenient to employ this formalism in building knowledge-based expert systems. A production rule is typically expressed in IF-THEN format; it may be represented as (see, e.g., Rich, 1983):

IF proposition 1
AND proposition 2
⋮ ⋮ ⋮
AND proposition m
THEN conclusion

Note that a conclusion is inferred only when all m propositions are satisfied.

In various applications a partial satisfaction of the premises is sufficient to lead to the corresponding conclusions. This typically involves assigning a level of satisfaction to each proposition. The minimum operator is a common technique employed for combining these levels of satisfaction (see, e.g., Zadeh, 1974). This often leads to a pessimistic evaluation and does not permit an evaluation in the absence of complete information (see, e.g., Shenoi et al., 1984). Meta-knowledge about the relative importance of each proposition to the conclusion may be employed to specify relative weights to these propositions (Shenoi et al., 1984). This necessitates a trade-off evaluation of the premise and, hence, the rule. The Sugeno integral (Sugeno, 1974) combines the levels of satisfaction of propositions

with their respective weights. It effectively emulates a trade-off procedure characteristic of human expert behavior. The resultant rule evaluation is balanced and well-rounded.

Much knowledge available for numerous domains, including scale-up of chemical processes, is of a qualitative nature. This is because human experts tend to express their knowledge subjectively (see, e.g., Buckley, 1984). Thus, it seems more appropriate to assign linguistic or qualitative relative weights as well as levels of satisfaction to the various propositions of a premise. Consequently, we may appropriately employ linguistic variables, such as "high" and "low", for evaluating production rules with the Sugeno integral technique.

TECHNIQUE

The premise X of a production rule is expressed as a set. For instance, a rule with m propositions may be stated as

IF X THEN conclusion

where

$$X = \{x_1, x_2, \ldots, x_m\} \qquad (4\text{-}1)$$

with x_i representing the i-th proposition in the premise X.

This is followed by assignment of relative weights to groups of propositions, or subsets Q of the premise set X. The relative weights are based on meta-knowledge about the production rule. The relative weight need be a monotonic

measure (Shenoi et al., 1984). This measure will be denoted by g(Q) where Q is a subset of X.

To evaluate a rule, a level of satisfaction $h(x_i)$ is assigned to each proposition x_i in the premise. It is performed as follows:

For a finite premise set X, let P(X) be the power set of X (i.e., set of all the sets formed by all combinations of the elements of set X). The rule evaluation, E(Q), may be defined by the Sugeno integral as

$$E(Q) = \int h(x) \circ g(.)$$

$$= \max_{F \in P(X)} \left(\min_{x_i \in F} (h(x_i)) \wedge g(Q \cap F) \right) \qquad (4\text{-}2)$$

Here, Q is a proper subset of X. In physical terms, F represents the view on the basis of which the evaluation is made.

The Sugeno integral, in the form given in Eq. (4-2), possesses interesting properties appropriate for the evaluation of production rules; this appropriateness can be justified by considering the intuitive aspects involved in the integration.

First, consider the term

$$\min_{x_i \in F} (h(x_i))$$

It represents the minimum and, hence, the most secure level of satisfaction provided by a view F. The most secure level of satisfaction provided by a view is combined with its relative importance

$g(Q \cap F)$

This combination is performed by the $\wedge$ (or Min) operator which serves to limit the evaluation obtained from a view to a value no greater than its importance.

Although F can be any element of the power set P(X), the assignment $Q \cap F$ limits the number of views on the basis of which the evaluation is made; therefore, F actually belongs to P(Q), the power set of Q. Thus, the evaluation is effectively performed only over Q, a proper subset of X. In practice, we may not have knowledge about all the premises in set X. In such a situation, this aspect allows the rule to be evaluated with incomplete knowledge.

The evaluation, i.e., the combination of the most secure level of satisfaction with its relative importance, is performed for all possible views $F \in P(Q)$. The best evaluation among those provided by all the views is regarded as the final evaluation for the rule; this is computed employing the Max operator.

In other words, the evaluation procedure consists of selecting the best or most optimistic outcome from the list of worst or most pessimistic outcomes afforded by the various views of a situation. This emulates a natural trade-off tendency of human experts.

Moreover, since our relative weight g is a monotonic measure, and since in general,

$$Q \subseteq X,$$

we have

$$g(Q) \leq g(X)$$

From Eq.(2), it is not difficult to obtain

$$E(Q) \leq E(X) \ , \forall Q \subseteq X \qquad (4\text{-}3)$$

From Eq. (4-3), which demonstrates monotonicity of the integral, we conclude that the smaller the set Q over which the integration is performed, the lower the value of the Sugeno integral. This implies that when relatively fewer premises and, hence, relatively fewer criteria are considered in an evaluation, the lower the strength of the conclusion. This is consistent with the tendency of human experts to be conservative in the absence of complete knowledge.

In an earlier work (Shenoi et al., 1984), the Sugeno integral technique was demonstrated with a chemical process design decision rule. It was deemed appropriate to assign relative weights to propositions from the closed interval [0,1]. Furthermore, propositions were permitted to adopt levels of satisfaction from the closed interval [0,1].

In most multi-criteria decision making problems, it is difficult to assign numbers of fractions, when there are a large number of alternatives and criteria to choose from (Buckley, 1984). Thus, assigning values in the interval of [0,1] to the relative weights and levels of satisfaction to propositions of a premise may not be always practically feasible.

As stated earlier, human experts tend to express their knowledge subjectively. It, therefore, seems more appropriate to resort to linguistic variables, such as "low" and "high", rather than numerical variables.

Towards this end we propose a linguistic scale

$$L_n = \{A_1, A_2, \ldots, A_n\} \tag{4-4}$$

L_n is a linearly ordered set with

$$A_1 < A_2 < \ldots < A_n$$

The A_i's are not numbers or fractions, but linguistic variables; they represent a qualitative notion of importance. Moreover, A_1 represents the linguistic concept of "null" importance, and A_n of "perfect" importance. Based on such a linguistic scale, the relative weights of a proposition may be assigned a linguistic variable, restricted by the following constraints;

(a) boundedness:

$$g(\Phi) = A_1 \text{ and } g(X) = A_n \tag{4-5}$$

(b) monotonicity:

$$\forall\, Q_1, Q_2 \in P(X), \text{ if } Q_1 \subseteq Q_2,$$

$$g(Q_1) \leq g(Q_2) \tag{4-6}$$

The complete premise X represents the total information available for evaluations. Thus, it is assigned a relative weight of A_n according to Eq. (4-5), i.e.,

$$g(X) = A_n$$

The empty set Φ contains no propositions; hence, it carries no relative weight according to Eq. (4-5), i.e.,

$g(\phi) = A_1$

The monotonicity constraint is logical to an intuitive understanding of combining numerous criteria. If Q_1 is a proper subset of Q_2, the set Q_1 contains at least one proposition less than the set Q_2. Consequently, Q_2 has to carry a relative weight equal to or greater than Q_1 in an evaluation.

For a production rule under consideration, the levels of satisfaction of each proposition may also be assigned based on linearly ordered linguistic scale L_n. In a practical implementation, this assignment would mostly be user input; nevertheless, the possibility of automatic assignment of levels of satisfaction for some propositions of some rules, based on previous conclusions, is an interesting one.

In Eq.(4-2),

$$\forall x_i \epsilon F,\ A_1 \leq h(x_i) \leq A_n \qquad (4\text{-}7)$$

and

$$\forall F \epsilon P(Q),\ A_1 \leq g(Q \cap F) \leq A_n \qquad (4\text{-}8)$$

From equations (4-2), (4-7) and (4-8), and the closure property of the Max and Min operators, it follows that

$$A_1 \leq E(Q) \leq A_n \qquad (4\text{-}9)$$

This implies that the production rule would evaluate to a point on the same linearly ordered linguistic scale L_n. This evaluation may be interpreted from the qualitative notion associated with the point.

The linguistic Sugeno integral evaluation possesses the following interesting property;

Property: Consider an m-proposition production rule with pre-determined g values, for all its views $F \in P(Q)$. Let $A_{i,j}$ be the level of satisfaction assigned to the j-th proposition, where A_i refers to a linguistic value on the n-point linguistic scale L_n. Also, let the rule evaluate to a value A_k on the same linguistic scale. Now, if the error in determining the levels of satisfaction is one unit, i.e., if one or more $h(x_i)$ are erroneously assigned a value $A_{(i-1),j}$ or $A_{(i+1),j}$, then the production rule also evaluates within an accuracy of one unit, i.e., it lies between $A_{(k-1)}$ and $A_{(k+1)}$.

Proof: If all values of a set were over-estimated by one unit, then their minimum or maximum would obviously be greater by one unit. Conversely, for similar under-estimation, the minimum or maximum would be less by one unit. Since the Sugeno integral involves only a combination of Min and Max operators, and a possibility exists of an error of one unit in levels of satisfaction, $h(x_i)$, (while $g(Q \cap F)$ are pre-determined or fixed), it follows that the maximum error in the final evaluation, E(Q), would be only one unit. □

The above property implies that if there exist errors of one unit in assigning levels of satisfaction to one or more propositions, based on a linearly ordered linguistic scale,

the maximum error in prediction of the strength of conclusion resulting from Sugeno integral evaluation would also be one unit on the same linguistic scale. Thus, fineness of judgement is not essential while assigning satisfaction levels, which in most practical implementations would be inputs from the user, who may be inexperienced. However, the analysis assumes that the assignment of relative weights to different views is correct. This implies that the Knowledge Engineer should be able to extract correct information from the domain expert. This would be more or less the case, if the Knowledge Engineer had some background in the domain of interest.

For practical implementation, it is essential to determine what value of n should be used for the n-point linguistic scale. If n is chosen to be relatively small, i.e., less than or equal to 5, the error introduced through judgmental differences would be magnified. At the other extreme, if n is chosen to be excessively large, e.g., more than 12, it would be frustrating to both the Knowledge Engineer as well as the end-user. Such a scale would imply being able to choose from a large number of linguistic points. First, it would be a difficult task for the Knowledge Engineer to extract such precise relative weights from either interviews with domain experts or review of available domain literature. Second, the user would also be unable to distinguish between a large number of linguistic

variables when making a choice for the questions asked; thus, the user would be likely to commit an error of more than one unit in judgement.

From a practical point of view, a value of 7 to 9 for n, seems favorable. In particular, the use of a linguistic scale consisting of 9 linearly ordered linguistic variables is suggested. Thus, in our case, n=9, with

$$L_9 = \{A_1, A_2, \ldots, A_9\}'$$
$$= \{Z, VL, L, ML, M, MH, H, VH, P\} \quad (4\text{-}10)$$

Here, the symbols have a semantic value as follows:

Z = Zero	VL = Very Low	L = Low
ML = Medium Low	M = Medium	MH = Medium High
H = High	VH = Very High	P = Perfect

If the linguistic points ML and MH were dropped, it would result in a 7-point scale. However, it is suggested that these points be retained; when humans think a criteria is of average importance, they do possess a notion of whether it is of less than average or more than average importance.

APPLICATION

Most commercial fluidized-bed reactors are designed by scaling up laboratory-scale reactors (see, e.g., Matsen, 1985). The widely-used similarity principle of scale-up involves establishing relationships between fluidized beds of different sizes, while maintaining the governing dimensionless groups constant (see, e.g., Trambouze, 1977).

Fluidization, being an extremely complex phenomenon, involves a large number of governing groups. In reality, it is impossible to maintain all of them constant. However, not all groups have the same importance in different situations; this makes it possible to weigh the effect of various criteria on these groups. Thus, fluidized-bed reactor scale-up is an instance of a multi-criteria decision making problem. It lends itself to the qualitative Sugeno integral technique discussed in the preceding section.

Set of Rules

In Chapter 2, an exhaustive review of the available domain literature in the field of fluidized-bed reactor scale-up has been performed. A critical analysis of this literature in chapter 3 has led to identification of the various dimensionless groups that need be maintained constant in scale-up. This enables us to formulate the following eight rules for fluidized-bed reactor scale-up.

Rule I

IF Fluidized-bed is operating in viscous limit [x_1]
AND Heat and Mass transfer are important [x_2]
AND Particle size employed is small [x_3]
THEN Maintain *Reynolds number* constant.

Rule II

IF Heat transfer is important [x_1]
AND Particle size is large (Geldart's Group D) [x_2]

THEN Maintain *Archimedes number* constant.

Rule III

IF Superficial fluid velocity is low [x_1]

AND Beds are slugging [x_2]

THEN Maintain *Linear dimension ratio* constant.

Rule IV

IF Fluidized bed is operating in inertial limit [x_1]

AND Operating pressure is high [x_2]

AND Particle size employed is small [x_3]

THEN Maintain *Solid-to-fluid density ratio* constant.

Rule V

IF Reaction order is high [x_1]

AND Superficial fluid velocity is low [x_2]

AND Reaction rate is fast [x_3]

THEN Maintain *Bubble phase gas fraction* constant.

Rule VI

IF Reaction rate is slow [x_1]

AND Number of mass transfer units is between 1 and 8 [x_2]

THEN Maintain *Number of reaction units* constant.

Rule VII

IF Reaction rate is fast [x_1]

AND Number of reaction units is very large [x_2]

THEN Maintain *Number of mass transfer units* constant.

Rule VIII

IF Number of mass transfer units is between 1 and 8 [x_1]

AND Number of reaction units is very small [x_2]

THEN Maintain *Number of mixing units* constant.

Table 4-1 shows the relative weights assigned to the various views of the propositions of each of these rules. The weights are assigned based on the linearly ordered nine-point linguistic scale.

Evaluation of Rule Set

Consider the following laboratory conditions. Particles with a diameter of 100 μm diameter and a density of 1,200 kg/m^3, belonging to Geldart's Group A powder type, are fluidized in a laboratory-scale fluidized bed. The density and viscosity of the fluidizing gas are 1.3 kg/m^3 and .02 cp, respectively. The minimum fluidization velocity and operating superficial velocity are 0.5 m/s and 1.8 m/s, respectively. The aim is to conduct a relatively fast gas-solid first order reaction; thus, mass transfer considerations are essential. The laboratory-scale fluidized-bed reactor is operated at ambient conditions; thus, heat transfer considerations are of little or no significance. The Reynolds number in the laboratory-scale bed is calculated to be about 12; this implies that the bed is operating in the intermediate limit, but very close to the viscous limit. Also, the Number of reaction units and the Number of mass transfer units are 40 and 4, respectively.

Table 4-2 shows the assignment of the levels of satisfaction $h(x_i)$ to the various propositions of each rule, based on above data.

Applying Eq. (4-2) to the values of relative weights and levels of satisfaction in Tables 1 and 2, respectively, we can obtain the final qualitative evaluation of each conclusion. This is shown in Table 4-3.

Thus, a qualitative ranking of the various criteria, i.e., dimensionless groups to be maintained invariant, is obtained from this evaluation. Therefore, the designer should try to maintain the groups with relatively higher importance constant in scale-up. The groups with average importance may be maintained approximately constant within acceptable limits. The groups with relatively lower importance, may be neglected from consideration.

Analysis of Rule I

Figure 4-1 shows the effect of levels of satisfaction of the three propositions of Rule I, on the strength of its conclusion; this is achieved through nine plots each keeping $h(x_1)$ constant and varying the other two levels of satisfaction, i.e., $h(x_2)$ and $h(x_3)$. The strength of the conclusions has been calculated by coding Eq. (4-2) into a simple Pascal program. It is enlightening to note the three-dimensional clusters formed by placing the nine plots of $h(x_1)$=Z,VL,L,...,P on top of each other; they serve to

provide a visual understanding of the relative insensitiveness of the evaluation technique to minor judgmental errors.

For illustration, let us consider a situation in which uncertainty exists in assigning the levels of satisfaction to the propositions of Rule I. Suppose that the user is uncertain whether to assign VL or L to $h(x_1)$, H or VH to $h(x_2)$ and ML or M to $h(x_3)$. This would result in a total of eight possible combinations of the various levels of satisfaction. Table 4 shows the evaluation of the strength of conclusion for all these combinations. The evaluation is either H or VH for all cases.

Consider a fluidized-bed reactor operating in the inertial limit, but very close to the intermediate region. Thus, the level of satisfaction $h(x_1)$ = ML. Also, the system involves almost no heat and mass transfer. Then $h(x_2)$ = VL. Moreover, the particle size of the solids used is very small; consequently, $h(x_3)$ = VH. We refer to the plots in Fig.4-1. to determine the strength of conclusion for these levels of satisfaction. We find it to be M or "Medium." This implies the conclusion is of medium or average importance for such a situation. This matches our intuitive reasoning. The more than average (MH) important first proposition has a less than average (ML) level of satisfaction and would afford an average contribution to the conclusion. Since, the very highly (VH) important second

proposition has a very low (VL) level of satisfaction, it would have a negligible contribution to the conclusion. The third proposition has average (M) importance, and has a very high (VH) level of satisfaction; it would have an average contribution to the conclusion. Intuitively, knowing that a combination of any two propositions has a high to very high (H to VH) relative weight, a human expert would assign average importance to the conclusion. This feature would enable us to implement a suitable explanation facility about the reasoning of the Expert System.

DISCUSSION

The Sugeno integral combines the level of satisfaction of the premises with their respective weights; it effectively emulates a trade-off procedure intrinsic to human problem solving and decision making. This technique can be employed effectively within a production-rule formalism natural to multi-criteria decision making problems.

Since most domain knowledge and natural thinking is qualitative, it is appropriate to assign linguistic relative weights as well as linguistic levels of satisfaction. This is successfully achieved by employing a suitable linearly ordered linguistic scale; specifically, a nine-point linguistic scale has been suggested. The semantic

interpretation of the points on this scale is also clarified.

The results obtained through the qualitative Sugeno integral evaluation technique form clusters. Thus, fineness of judgement is not required by the user of a rule-based system utilizing this technique as its reasoning mechanism. This feature is formally proposed as a property which may be stated as: If there errors of one unit occur in assigning levels of satisfaction to one or more propositions, based on a linearly ordered linguistic scale, the maximum error in predicting the strength of conclusion with the Sugeno integral evaluation would also be one unit on the same linguistic scale.

The intuitive nature of the Sugeno integral evaluation would allow a suitable explanation facility for the conclusions arrived at by a rule-based Expert System, based on the Sugeno integral technique.

The significance of the present work is evident when we consider the complexity of fluidization accompanied by chemical reaction. To cope with the virtual impossibility of maintaining a large number of governing dimensionless groups invariant, scale-up experts employ ad-hoc strategies based on extensive experience in arriving at a ranking of the groups to be maintained invariant. The proposed technique relying on non-additive evaluations on a linguistic scale is a formal, albeit flexible methodology

that promises to be especially effective for scale-up and design.

CONCLUSIONS

The Sugeno integral technique is successfully employed as a qualitative trade-off strategy for scale-up of fluidized bed reactors. Scale-up rules have been proposed based on available domain knowledge. The evaluation of the scale-up rules, based on the relevant process conditions, gives rise to a ranking of the dimensionless groups to be maintained invariant; such a ranking allows the trading-off of these dimensionless groups.

NOTATION

A_j = j-th point on the linguistic scale

E(Q) = partial evaluation of rule

E(X) = evaluation of rule

F = view

g = relative weight

$h(x_i)$ = level of satisfaction of i-th proposition

H = High

L = Low

L_n = n-point linguistic scale

M = Medium

MH = Medium High

ML = Medium Low

P = Perfect

P(X) = power set of set X

Q = partial premise set

VH = Very High

VL = Very Low

x_i = i-th proposition of a premise

X = premise set

Z = Zero

ϵ = belongs to

ϕ = empty set

$\wedge$ = minimum operator

$\forall$ = for all values of

$\subset$ = improper subset of

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Table 4-1. Linguistic Relative Weights for Fluidized-Bed Reactor Scale-Up Rules.*

g(Q∩F) \ Rule #	I	II	III	IV	V	VI	VII	VIII
$g(\Phi)$	Z	Z	Z	Z	Z	Z	Z	Z
$g(\{x_1\})$	MH	H	M	MH	MH	H	MH	H
$g(\{x_2\})$	VH	L	H	M	M	M	M	M
$g(\{x_3\})$	M	na	na	M	H	na	na	na
$g(\{x_1,x_2\})$	VH	P	P	H	H	P	P	P
$g(\{x_1,x_3\})$	H	na	na	H	VH	na	na	na
$g(\{x_2,x_3\})$	VH	na	na	H	H	na	na	na
$g(\{x_1,x_2,x_3\})$	P	na	na	P	P	na	na	na

*Note: 'na' implies not applicable.

Table 4-2. Assignment of Levels of Satisfaction.

Rule # \ $h(x_1)$	$h(x_1)$	$h(x_2)$	$h(x_3)$
I	MH	MH_*	H
II	VL	Z_{**}	-
III	L	Z	-
IV	VL	VL	H
V	VL	L	VH
VI	VL	P	-
VII	VH	VH	-
VIII	P	VL	-

*Determined to have Zero satisfaction level.
**No information available for this premise.

Table 4-3. Qualitative Evaluation of Fluidized-Bed Reactor Scale-Up Rules.

Rule #	E(Q)	To maintain constant	Importance
I	MH	Reynolds number	Medium High
II	VL	Archimedes number	Very Low
III	L	Linear dimension ratio	Low
IV	M	Solid-to-fluid density ratio	Medium
V	H	Bubble phase gas fraction	High
VI	M	Number of reaction units	Medium
VII	VH	Number of mass transfer units	Very High
VIII	H	Number of mixing units	HIgh

Table 4-4. Analysis of Rule I.

Combination #	1	2	3	4	5	6	7	8
$h(x_1)$	VL	VL	VL	VL	L	L	L	L
$h(x_2)$	H	H	VH	VH	H	H	VH	VH
$h(x_3)$	ML	M	ML	M	ML	M	ML	M
Evaluation E	H	H	VH	VH	H	H	VH	VH

Fig. 4-1. Analysis of Rule I.

Chapter 5

QUALITATIVE SIMULATION OF BUBBLE SIZE DISTRIBUTION

In modeling chemical processes, heuristic judgement and empirical skills are often required. In practice, this task is performed frequently based on incomplete and uncertain knowledge. The developing field of qualitative physics seems to be a plausible domain to explore for such modeling purposes. Qualitative physicists propound that the description of a system's behavior must be derivable from the structure of the system (see, e.g., Bobrow, 1984). Thus, it should be possible to start with a structural description of the system and predict a change in its parameters in the future; this is termed as qualitative simulation.

The technique of qualitative simulation allows prediction of process behavior from incomplete, uncertain physical description. Physical laws acquired from domain knowledge can be effectively portrayed as a production system (Voller and Knight, 1986). A production system consists of a set of rules that would describe the principles governing a process or phenomenon. The rule base so formed would represent a qualitative model for the process. The rules linked to a model are generated by considering the process model to be a 'black box' number generator (see, e.g., Voller and Knight, 1986). The validity of the resultant model depends on the power of the

rules to screen out erroneous numbers and retain the correct ones. The usage of the term "black box" is discouraged in this context. Since the method uses knowledge about the process to sieve out the incorrect random numbers, it should be considered a "gray box" approach. The method could appropriately be termed as the "gray box random number generator" methodology.

PREDICTION OF BUBBLE SIZE DISTRIBUTION

In bubbling fluidized beds, gas usually flows in the form of bubbles. The bubbles formed are varying in size. In general, the bubble size increases with increasing bed height. Thus kinetic models which assume a constant bubble size, e.g., the bubbling bed model of Kunii and Levenspiel (1977) may not be sufficiently accurate. This necessitates a knowledge of the bubble size distribution in the fluidized bed.

To include the variation in bubble size with bed height, Kato and Wen (1969) have proposed the bubble assemblage model. The important assumptions of this model include the following;

(a) The fluidized bed is divided into N compartments-in-series; the height of each compartment is equal to the size of the bubble at the corresponding bed height.

(b) Bubbles are assumed to be spherical in shape.

(c) Bubbles are considered to grow continuously in size until they reach the maximum stable size based on either the terminal velocity or the bed diameter.

In the bubble assemblage model, the bubble diameter is represented approximately as a function of height as

$$D_B = 0.14\ \rho_s d_p \left[\frac{U}{U_{mf}}\right] h + D_{BO} \qquad (5\text{-}1)$$

where the initial bubble diameter D_{BO} is as given by Cooke et al. (1968), i.e.,

$$D_{BO} = \left[\frac{6(U - U_{mf})}{\pi\ n_o \sqrt{g}}\right]^{-0.4} \qquad (5\text{-}2)$$

Gray Box Random Number Generation

The bed is assumed to be divided into N compartments such that the height of each compartment is equal to the bubble size at this height. If we had no knowledge about the phenomenon, any set of random bubble sizes would be acceptable. We know, however, that the bubble sizes have to lie between the limiting minimum and limiting maximum diameters. The limiting minimum diameter is dependent on the distributor hole size and configuration. The limiting maximum diameter depends upon the stability of the bubble from the viewpoint of either the terminal velocity or the diameter of the fluidized bed. Thus only those random bubble sizes located between these two extremes should be chosen. It should be noted that the sum of the N bubble

diameters obtained should be nearly equal to the height of the fluidized bed. Furthermore, our sense of judgement informs us that no two bubble sizes so obtained should be very close to each other. Again, as the bubble size increases with the height, the random bubble sizes obtained have to be arranged in ascending order with increasing height.

Expert Rule Base

Based on the knowledge of the bubbling phenomenon in a fluidized bed, presented in the preceding section, the following expert rule base is proposed.;

Rule 1 Generate N bubble sizes.

Rule 2 No bubble size may be greater than the limiting maximum bubble diameter.

Rule 2a The maximum bubble size should be very close to the limiting maximum diameter.

Rule 3 No bubble size may be less than the limiting minimum bubble diameter.

Rule 3a The minimum bubble size should be very close to the limiting minimum diameter.

Rule 4 The sum of the N bubble sizes should nearly equal to the bed height.

Rule 5 No two bubble sizes may be very close to each other.

Rule 6 The bubble sizes should increase monotonically with increasing height.

This rule base represents the skeleton of a qualitative model for prediction of the bubble size distribution in a bubbling fluidized bed. Its exact structure would depend on the implementation.

To demonstrate the utility and importance of the technique and the accuracy of the qualitative model, a simple FORTRAN program to implement the rules has been employed. The program uses a conventional technique to generate random numbers which are converted to the bubble size range. If the rules are not satisfied, the random numbers are regenerated until a size distribution satisfying all the rules is obtained.

The proposed rules contain subjective terms like "nearly equal" and "very close." In the current implementation, these terms have been pre-evaluated based on our experience and judgement; for instance, in Rule 4, a value of 0.77m to 0.83m is considered "nearly equal" to a bed height of 0.8m. It is possible to interpret these terms employing sets that do not have a crisply defined membership; such sets are termed "fuzzy sets" and the reasoning on computers resorting these fuzzy sets is considered to mimic human reasoning (see, e.g., Zadeh, 1987).

Comparison with Existing Model

For the following set of data representing the operating conditions and bed characteristics;

$H = 0.8$ m

$n_o = 1000\ /m^2$

$d_p = .0005$ m

$\rho_s = 1400\ kg/m^3$

$U_{mf} = 0.05$ m/s

and

$U = 0.18$ m/s

Kato and Wen (1969) have obtained from equations (5-1) and (5-2), respectively,

$D_{BO} = 0.023$ m

and

$D_{BH} = 0.28$ m

These two values are also used as the limiting minimum and maximum diameters in the present qualitative model. For the qualitative model (QM) the bed has been assumed to be divided into 5 compartments.

The bubble size distribution predicted by the bubble assemblage model (BAM) is presented in Table 5-1. The qualitative simulation has been performed for five different seed inputs to the gray box random number generator program. The bubble size distribution for these five runs is listed in Table 5-2. Note that some of the values for bed height

exceed 0.8 m, as Rule 4 is involved only in checking for "very close" to the bed height.

These five distributions are compared in Fig. 5-1. It is observed that for different runs of the qualitative simulation, the prediction is sufficiently close. Moreover, they compare well with the cubic regression plot of the bubble assemblage model values given in the same figure.

It is interesting to note that while any deterministic mathematical model, e.g., the bubble assemblage model, predicts a single value of the bubble diameter at a given height, the qualitative model is capable of predicting a range of bubble diameters at a given height. In practice, there exists a range of bubble diameters at any given height.

Comparison with Experimental Data

Cooke et al. (1968) have presented experimental data, obtained with coal particles, for variation of bubble diameter with height for the following set of conditions;

$H = 0.8$ m

$n_o = 350 /m^2$

d_p = -10 BSS mesh (-0.0017 m)

$d_o = 0.0032$ m

$\rho_s = 1500$ kg/m^3

$U_{mf} = 0.05$ m/s

and

$$U = 0.18 \text{ m/s}$$

For this set of data, the limiting minimum bubble diameter is taken to be the size of the distributor hole; this information is required for the qualitative model. For lack of a better estimate, the limiting maximum bubble diameter is taken to be the diameter at the top of the bed, determined experimentally. The resultant values of the diameters are:

$$D_{BO} = 0.0032 \text{ m}$$

$$D_{BH} = 0.279 \text{ m}$$

The experimentally obtained values of the bubble size distribution data are listed in Table 5-3. The bubble size distributions obtained for five different seed inputs to the gray box random number generator program are presented in Table 5-4. For the qualitative model (QM), the bed has been assumed to be divided into 5 compartments. Again,some values of bed height exceed 0.8 m because of the nature of Rule 4.

A comparative plot of these distributions is drawn in Fig. 5-2. Again, the predictions for different runs of the qualitative simulation are sufficiently close;they compare well with Cooke's experimental data, as the predictions lie within 99% confidence limits of these experimental values (see Fig.2).

The qualitative model slightly overestimates the experimental values. Nevertheless, the model is

sufficiently satisfactory, especially considering the random and stochastic nature of bubble formation and motion in a fluidized bed. Moreover, overestimation of the bubble sizes renders the qualitative model conservative with respect to prediction of reactant conversion and bed stability; specifically, a larger bubble size would lead to a lower conversion, and a larger bubble size also would imply lower stability. Thus, the resultant reactor design based on the present qualitative model would be conservative.

CONCLUSIONS

In a bubbling fluidized bed, the bubble size varies with the bed height. The reactant conversion in a fluidized bed and the bed stability are functions of the bubble size. Thus, there is a need to predict the bubble size distribution. The gray box random number generator methodology has been successfully employed to predict this distribution. The results of qualitative simulation compare favorably with one another for different values of the input seed to the program. Furthermore, the prediction is very close to that estimated by the bubble assemblage model, as well as to the available experimental data.

The qualitative model slightly overestimates the experimental values. Although the expert rule base could be refined with further insight into the problem, it is deemed satisfactory in its present state. Moreover, predicting

higher bubble sizes than those existing in the actual bed implies a conservative estimate.

The encouraging results suggest that the technique, besides being utilized for the purpose of predicting bubble size distribution in a bubbling fluidized bed, could be utilized for other similar problems. Processes with a stochastic behavior are well-suited to this methodology, as it offers near solutions with a fast computation speed.

Within the area of bubble size distribution in a fluidized bed, additional constraints may be added to the problem description. For instance, the volume of gas passing through the bubble phase should be consistent with the bubble sizes generated and their frequency of occurance. Further work may be fruitfully conducted in this direction. To demonstrate the utility of the technique, the rules have been implemented in a FORTRAN program. This implementation utilizes experience and judgement to evaluate fuzzy terms. It would be worthwhile to develop a linguistic interpretation resorting to fuzzy logic for these rules, which could then be implemented in a suitable functional language, e.g., LISP.

NOTATIONS

d_o = size of the distributor hole [m]

d_p = particle diameter [m]

D_B = bubble diameter [m]

D_{BO}	=	initial bubble diameter	[m]
D_{BH}	=	bubble diameter at height H	[m]
g	=	acceleration due to gravity	[m/s^2]
h	=	vertical distance from the distributor	[m]
n_o	=	number of distributor holes per unit area	[$1/m^2$]
U	=	superficial gas velocity	[m/s]
U_{mf}	=	superficial gas velocity at minimum fluidization	[m/s]
ρ_s	=	solid density	[kg/m^3]

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Table 5-1. Prediction by BAM for experimental conditions of Kato and Wen (1969)

Height, h m	Bubble diameter, D_B m
0.0	0.023
0.2	0.091
0.4	0.148
0.6	0.204
0.8	0.280

Table 5-2. Prediction by QM for experimental conditions of Kato and Wen (1969)

Run #1		Run #2		Run #3		Run #4		Run #5	
h m	D_B m	h m	D_B m	h m	D_B m	h m	D_B m	h m	D_B m
0.037	0.037	0.032	0.032	0.030	0.030	0.034	0.034	0.038	0.038
0.122	0.085	0.145	0.113	0.153	0.123	0.139	0.105	0.134	0.096
0.314	0.192	0.327	0.182	0.315	0.162	0.312	0.173	0.330	0.196
0.528	0.214	0.537	0.210	0.553	0.238	0.528	0.216	0.557	0.227
0.791	0.263	0.814	0.277	0.822	0.269	0.808	0.280	0.828	0.271

Table 5-3. Experimental data for experimental conditions of Cooke et al. (1968)

Height, h m	Bubble diameter; D_B m
0.0	0.036
0.2	0.102
0.4	0.180
0.6	0.220
0.8	0.279

Table 5-4. Prediction by QM for experimental conditions of Cooke et. al. (1968)

Run #1		Run #2		Run #3		Run #4		Run #5	
h (m)	D_B (m)	h (m)	D_B (m)	h (m)	D_B (m)	h (m)	D_B (m)	h (m)	D_B (m)
0.022	0.022	0.022	0.022	0.006	0.006	0.030	0.030	0.029	0.029
0.140	0.118	0.137	0.115	0.107	0.101	0.114	0.084	0.129	0.100
0.326	0.186	0.310	0.173	0.305	0.198	0.289	0.175	0.306	0.177
0.527	0.201	0.545	0.235	0.526	0.221	0.521	0.232	0.553	0.227
0.786	0.259	0.809	0.264	0.804	0.278	0.782	0.261	0.790	0.257

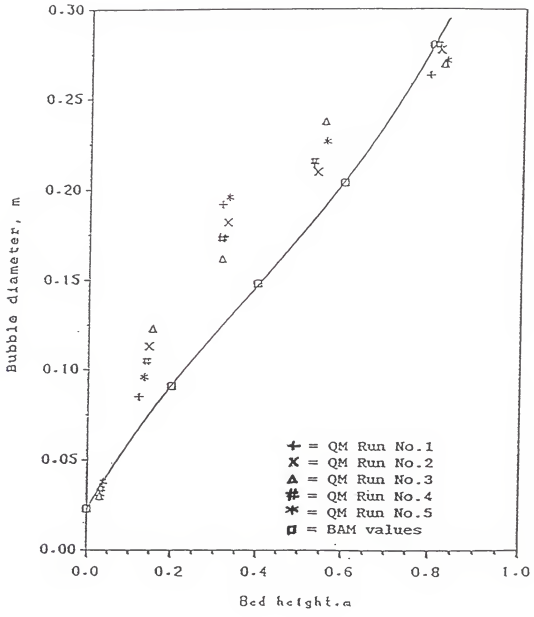

Fig. 5-1. Comparison of the bubble assemblage model with the qualitative model.

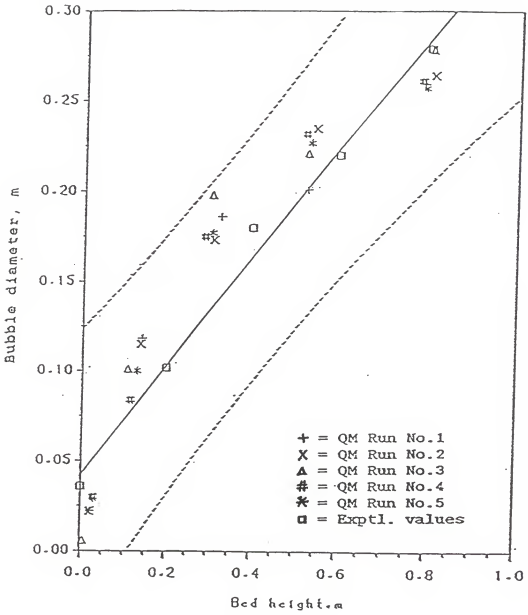

Fig. 5-2. Comparison of experimental data with the qualitative model.

Chapter 6

CONCLUSIONS AND RECOMMENDATIONS

Due to the lack of a highly reliable theory of fluidization, the modeling, scale-up and design of fluidized-bed reactors is an indecisive endeavor. The available knowledge in this domain is often uncertain, approximate, incomplete and qualitative in nature. Recent advances in the developing field of artificial intelligence offer an attractive alternative to express and reason with such information.

From the exhaustive review and critical analysis of the available literature for scaling up fluidized-bed reactors, four kinds of similarities have been identified. Moreover, a large number of dimensionless groups that need be maintained constant in scaling up such reactors have been identified.

In reality, it is impossible to maintain the large number of dimensionless groups identified constant in scale-up. Nevertheless, it is possible to weigh the effect of different criteria on the various groups to determine their importance to a particular or specific case. The Sugeno integral effectively emulates a trade-off procedure intrinsic to human problem solving and decision making; a technique based on this non-additive integral employing a linguistic scale has been successfully employed as a qualitative trade-off strategy for scale-up of fluidized-bed

reactors. Scale-up rules have been proposed based on available domain knowledge. The evaluation of the scale-up rules, based on available process conditions, gives rise to a ranking of the dimensionless groups to be maintained invariant; such a ranking is important to the trading-off of these dimensionless groups.

The basic elements of a modeler's knowledge can be effectively portrayed as a set of production rules; such production rules corresponding to a process model can be developed using a gray box random number generator methodology. This method has been applied to predict the bubble size distribution in a fluidized bed. The distribution obtained from the resulting qualitative model compares well with available experimental data as well as the distribution predicted by existing theory.

The following recommendations are suggested for future work. It is possible to build rules on top of the existing set of scale-up rules to include (a) powder classification and (b) slugging characteristics. The rule-based system may be suitably implemented employing a functional language like LISP. The "expert rule base" for qualitative simulation of bubble size distribution may be further improved by implementing a fuzzy interpretation of the non-crisp terms of the qualitative model. It is worthwhile to explore other areas, i.e., physico-chemical phenomena characterized by

random or stochastic behavior, for diversification of the proposed qualitative simulation technique.

The ultimate objective of this study was to contribute to the development of an intelligent expert system for fluidized-bed reactor design. Scale-up and modeling are significant activities in designing fluidized-bed reactors. The approximate and qualitative techniques suggested for this activities can be effectively incorporated and implemented in the overall expert system.

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FLUIDIZED-BED REACTOR DESIGN:
Approximate Reasoning and Qualitative Simulation

by

RIZWAN MITHANI

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Department of Chemical Engineering

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A study was undertaken to explore the application of artificial intelligence oriented reasoning for modeling, scale-up and design of fluidized-bed reactors. The study was contributory to the ultimate objective of developing an intelligent expert system for fluidized-bed reactor design.

The available contributions to the theory and practice of scaling up fluidized-bed reactors was exhaustively reviewed and critically analyzed. Four kinds of similarities have been identified; these include (i) hydrodynamic, (ii) chemical, (iii) geometric, and (iv) particle similarity. The significance and limitations of these contributions are compared with one another; moreover, an attempt has been made to resolve the contradictions among them. The various dimensionless groups that need be maintained constant in scaling up such reactors have been identified; these include Reynolds number [Re], Froude number [Fr], Archimedes number [Ar], linear dimension ratio (e.g., L/D), solid-to-fluid density ratio, bubble phase gas fraction, Number of reaction units [N_R], Number of mass transfer units [N_X] and Number of mixing units [N_D].

Based on the available domain knowledge, a number of production rules have been formulated; these rules specify the conditions necessary for maintaining a particular dimensionless group constant in scale-up. Since the conditions are not of equal importance in maintaining a dimensionless group constant, knowledge about the relative

importance of propositions has been employed in assigning relative weights to individual propositions and groups of propositions. Since, humans tend to express their knowledge in subjective terms, this assignment is based on a linearly ordered nine-point linguistic scale: {Zero, VeryLow, Low, MediumLow, Medium, MediumHigh, High, VeryHigh, Perfect}. The levels of satisfaction for each proposition are assigned based on the same linguistic scale. The evaluation of the rules has been performed by employing the non-additive Sugeno integral. It has been demonstrated that the technique employed is appropriate for development of a rule-based Expert System for fluidized-bed reactor scale-up.

Prediction of the bubble size distribution is a significant part of modeling fluidized-bed reactors. From a qualitative description of bubble formation in fluidized beds, an 'expert rule base' has been proposed to represent a qualitative model of the phenomenon. The gray box random number generator method has been proposed and employed to predict the bubble size distribution; this is implemented in FORTRAN. The resultant distribution compares well with the existing bubble assemblage model as well as the available experimental data.