

Modeling the Bubbling Fluidized Bed Reactor, BFB.
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During the Second World War the US had an urgent need to produce enormous quantities of aviation gasoline. Fine particle fluidization (the FCC process) was proposed, was chosen, commercial plants were built chop-chop, and was wildly successful. Interestingly, all were built without any basic information on flow, heat transfer, mass transfer, reaction behavior, and other contacting phenomena in these units. After the war news of this new G/S contacting method was made public, and this spurred the research community to explore its properties and its unique features.

The first phenomenon studied was the very simplest, the heat transfer rate between particles and the fluidizing gas. Figure 1 is a tabulation of these early research publications, and there were at least 23 until 1965. These come from all over the world - the US, Europe, Russia, and Japan.

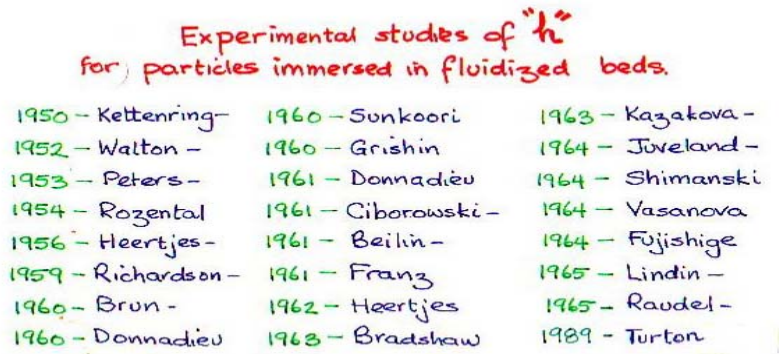


Figure 1.

These researchers measured entering and leaving gas temperatures, and on assuming plug flow or mixed flow of gas in the bed calculated values for "h". Figure 2 shows their resulting correlations on a Nu vs. Re plot.

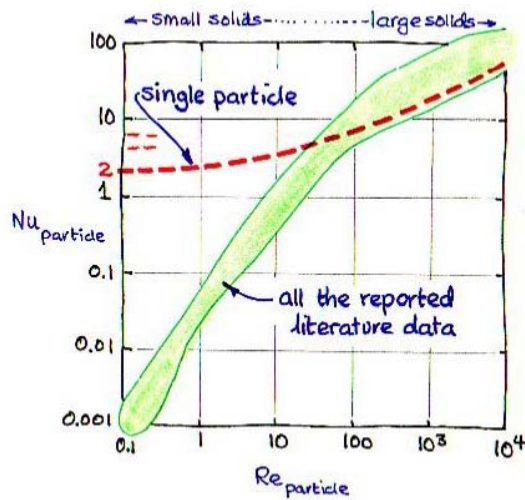


Figure 2.

This figure also shows some theoretical estimates for “h”, as well as the correlation for single particles falling through fluids. Note that the theoretical estimates all lay above the single particle correlation, while the experimental values all lay way below -- some by a factor of 1000 or more.

It is hard to understand why not one of the 23 experimenters questioned his low result. Wouldn't he suspect that in an environment containing many buffeting and colliding particles and much turbulence, that ‘h’ between particle and gas would be greater than for a single falling particle? Why didn't he ask these questions? What kind of a researcher was he?

He could have made a thought experiment to see whether his reported results were reasonable and made sense. Let us do that now. Imagine a bubbling fluidized bed of 100 μm copper particles all at 100 °C (see Fig. 3). Note, the particles have the same diameter as the hair on your head. Now introduce into the bed a single particle at 0 °C and ask how long it takes for the particle to heat up to 90 °C?

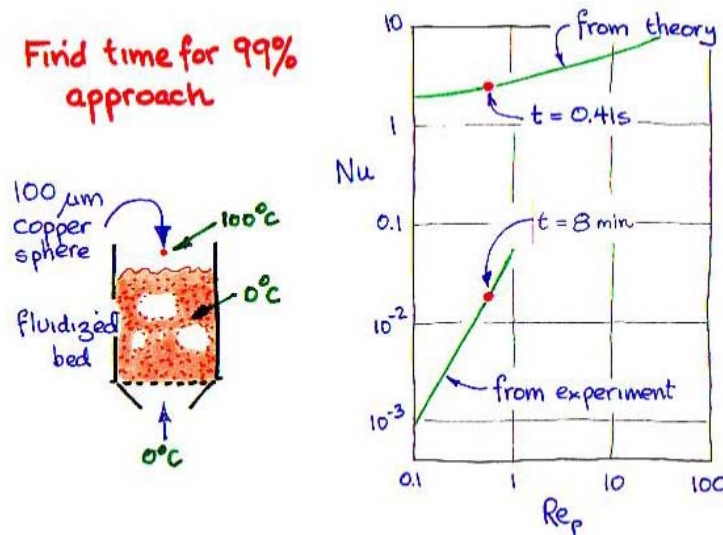


Figure 3.

Eight minutes or a quarter second --- what sounds more reasonable? Certainly not the 8 min. This typical example suggests that all 23 experimenters had made the same terrible mistake, and that all their results were wrong. What is the explanation for this? Let us explain.

Now for any process there are 4 interrelated quantities

- 1&2 The inlet and outlet flow conditions
- 3 The kinetics, including the heat and the mass transfer rates
- 4 The flow pattern in the vessel.

If you measure 1 and 2, then 3 and 4 are related. So if you make an error in 3 then 4 is also wrong. Here in these experiments, since the “h” value is way off this means that the flow model chosen (plug or mixed flow) is wrong. But what is it? Let us look into this problem.

Chemical Reactor: Plug Flow or Mixed Flow Model.

Numerous investigators have studied the behavior of solid catalyzed fluidized bed reactors. They measured the entering and leaving fluid compositions; they knew the reaction rate constant (the kinetics) so they could check the fit of this or that flow model.

Figure 4 shows that their results did not fit either the plug flow or mixed flow models, often behaving much worse than either,

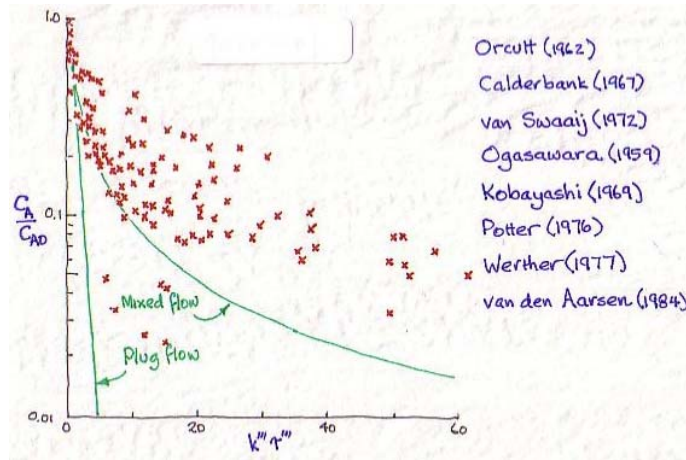


Figure 4.

This is consistent with the finding in heat transfer, in which the heat transfer rate is much lower than expected from either of these models.

So to conclude: the simple \$10 models of plug flow and mixed flow do not reasonably represent the flow of gas in fluidized beds, and can be off by a factor of as much as 10 000!

Arbitrary Two Region Flow Models.

Johnstone and his research group [1] said “Let’s LOOK at the BFB to see if there are any clues to this surprisingly bad behavior”. They noticed that the bed consisted of a dense region through which rose voids, which we call bubbles.

Johnstone’s group was the first to account for this, and this pointed to a new class of model, the 2-region 6-parameter model shown in Fig. 5.

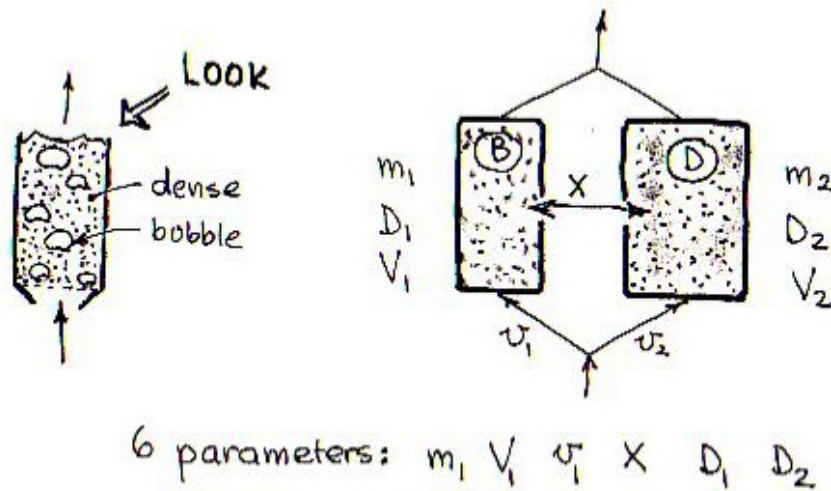


Figure 5.

Many special cases were proposed, and Fig. 6 illustrates 4 of these

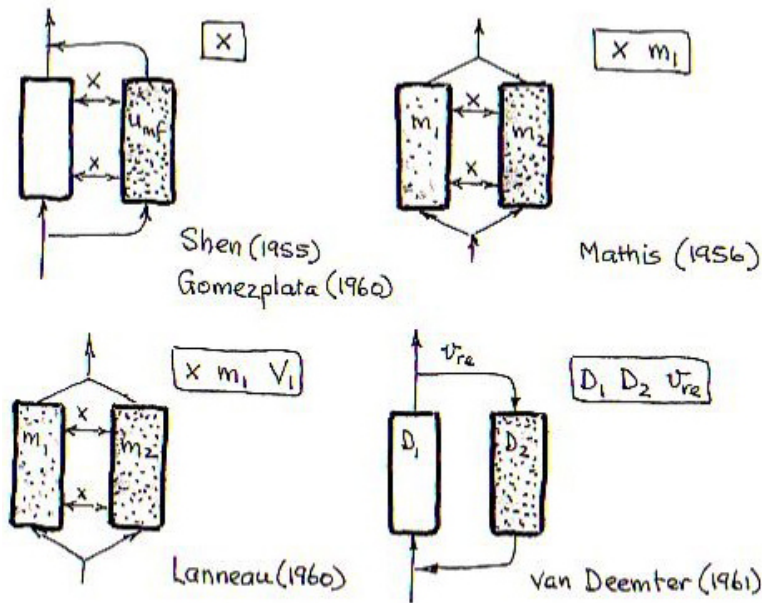
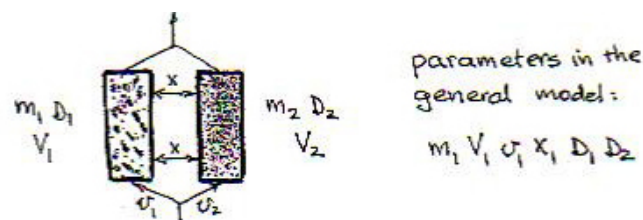


Figure 6.

Sketch (a) shows a one adjustable parameter model, sketch (b) shows a two parameter model, and sketches (c) and (d) show two different three parameter model. Note that sketches (a) and (d) assume that the bubbles are free of solids; sketch (d) shows no interchange between regions, and so on.

With so many alternatives available we are left with a whole basketful of flow models, at least 34 by 1970, which extrapolate differently. For example, of the three-parameter models, Shell (Amsterdam) chose sketch (d), while Shell (Baton Rouge) chose sketch (c). These two models are definitely contradictory, for example one says that the emulsion gas flows upward, the other says downward! Did this bother them? Not at all, because both these models fit the data.

Figure 7 shows other more complicated models. Exxon even said "We have the best mathematicians and the biggest computers in the business so we'll use the \$1000 six parameter model". The constants varied for their different units, and for their different feeds, whether from Venezuela, or Nigeria, etc. Some of their fitted volumes were negative, but it didn't matter because the fit to their data was wonderful.



Number of parameters used in the models

1 Shen	1 Orcutt	4 Mochi
1 Gomezplata	1 Lanneau	4 Mamuro
2 Mathis	1 Massimilla	
2 May	3 van Deemter	6 Exxon
2 Lewis	4 Kobayashi	

[from J.R. Grace C&P Symp. Ser. # 116 67 159 (1971)]

Figure 7.

Yes, with the proper choice of constants these 34+ models fit everything but predict nothing.

Discussion of Engineering Models.

Here are dozens of models, all contradictory, but all able to fit the data.

Doesn't that bother you? It does bother me, and leads me to ask, "What are the requirements of an engineering model?" I would like to forward three criteria:

- * First of all, the model must fit the data,
- * It must be extrapolatable, theoretically and/or (preferably) experimentally,
- * Its parameters must be reasonable from the physical point of view, and not be arbitrarily chosen to fit each specific situation.

Let me illustrate what I mean with a simple example. Suppose I give you the five data points shown in Fig.8

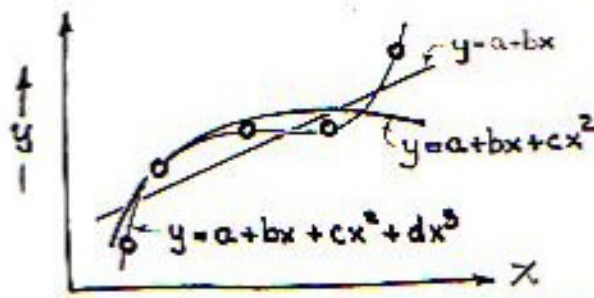


Figure 8.

First, second and third order polynomials would all satisfactorily fit the data. But to tell which more closely represents reality extrapolate the conditions and then see which model continues to fit the data. Figure 9 shows that at larger x values the y value of the cubic zooms up to infinity, the linear model predicts a modest rise in y value, while the quadratic predicts a decrease in y value. This would be a discriminating test for these models.

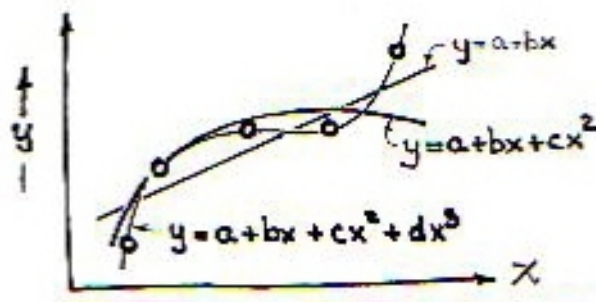


Figure 9.

Unfortunately no one tried widely different experimental conditions to test his fluidization model, so we are left with a whole basketful of models, all claiming to represent reality, but all making different predictions. Thus they are quite useless for scale up and design.

The Genius of Davidson.

At this point Davidson [2] said, "Let's not just LOOK at the fluidized bed and note the bubbles, let us try to use a bit of science to ANALYSE the behavior of the bubbles". He then invented the very simplest of models based on fluid mechanics. He assumed spherical bubbles free of solids in a bed whose solids moved out

of the way of the rising bubbles as an inviscid fluid, and where the gas flowed through the dense region as an incompressible viscous fluid.

At first thought you may think this as ridiculously crude, not even a \$10 model. But the consequences of this picture were magical, and when tested against experiments were spectacular.

I can't go into this development here, except to say that for fine particle beds bubbles rise as vortex rings, each surrounded by a thin cloud or 'halo' of circulating gas. The bubble gas in these fine particle beds remains segregated from the rests of the gas in the bed. For coarse particle beds the behavior is quite different. See Fig.10 for sketches of these two extremes.

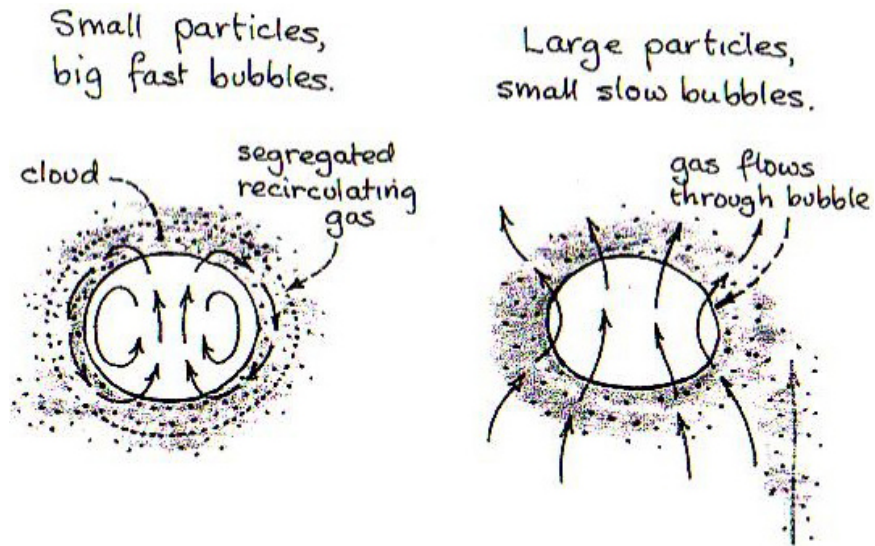


Figure 10.

With this breakthrough researchers stampeded to this concept, and developed all sorts of models. Figure 11 shows the five distinct choices available;

- * Spherical or non-spherical bubbles,
- * Bubbles followed by wakes or without accompanying wakes,
- * Bubbles constant in size, or growing in size, or having a size distribution, which changes with height in the bed.
- * Unchanging bubbles, or coalescing and splitting bubbles,
- * Assume that the bed consists of three regions - the bubble, the cloud and emulsion - or else combine bubble and cloud, or cloud and emulsion to give two region models.

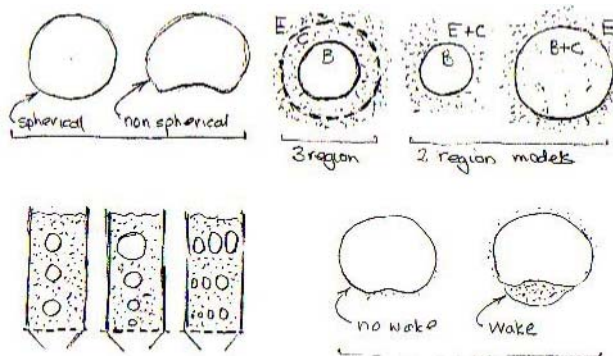


Figure 11.

Figure 12 shows some of the combinations chosen.

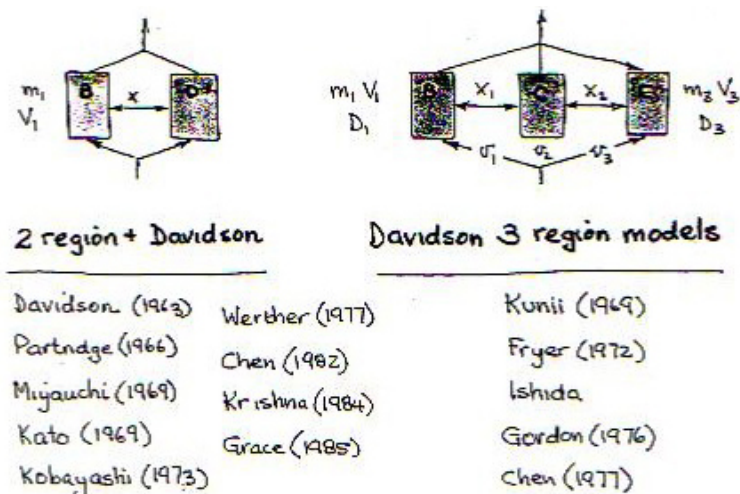


Figure 12.

Which of these models should we use? Bubbles certainly are not spherical, they split apart, they coalesce and they certainly are not uniform in size. But it does not make sense to incorporate into model complications that cannot be measured. No, at this point we should heed Einstein's admonition on model building

"Keep things as simple as possible, but not simpler"

With this in mind we choose the three-region flow model of Kunii and Levenspiel [3 and 4], which contains just one size of bubble, shown in Fig.13. The one parameter of this model can be observed and measured. It is the bubble size.

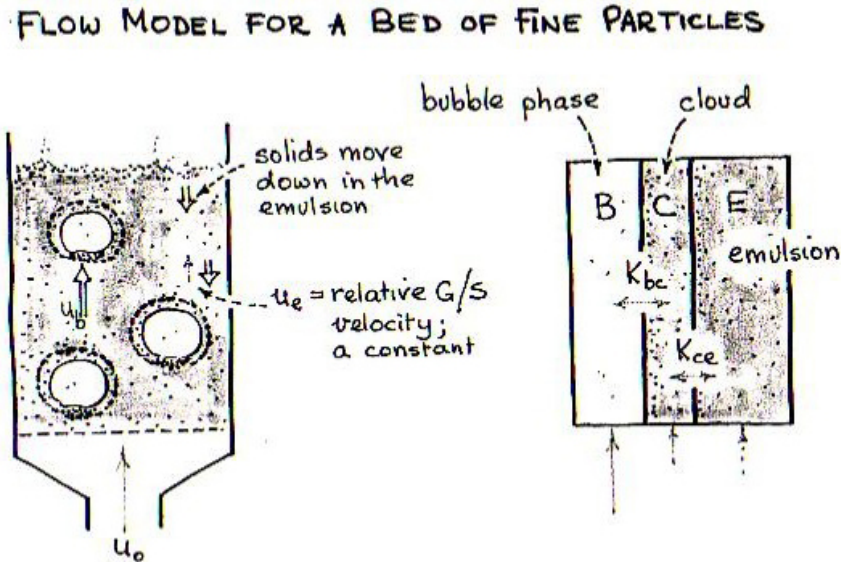


Figure 13.

The chemical conversion for this model can be determined without computers. But does this model represent an engineering model? The definitive answer to this question requires that we run experiments using different bubble sizes, and see how the conversion changes with bubble size. Since no one has done this we turn to the theoretical estimate.

For this consider the example of Fig. 14, a bed 2m in diameter 2m high containing 7 tons of catalyst with rate constant shown.

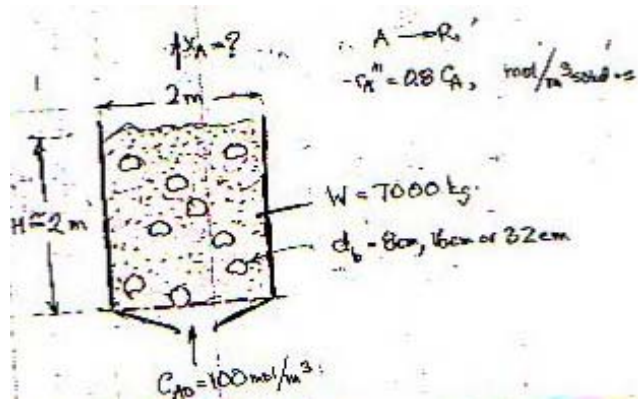


Figure 14.

Let us see what conversion this model predicts for different bubble sizes, and let us see if the predictions are reasonable. We find:

- *For no bubbles (a packed bed) 95% conversion
- * As bubbles grow in size from 8 to 16 to 32 cm conversion decreases to 84%, to 59% and to 32%. This is shown in Fig. 15.

Thus larger bubbles give more gas by passing, and thus lowers the gas conversion. This seems reasonable.

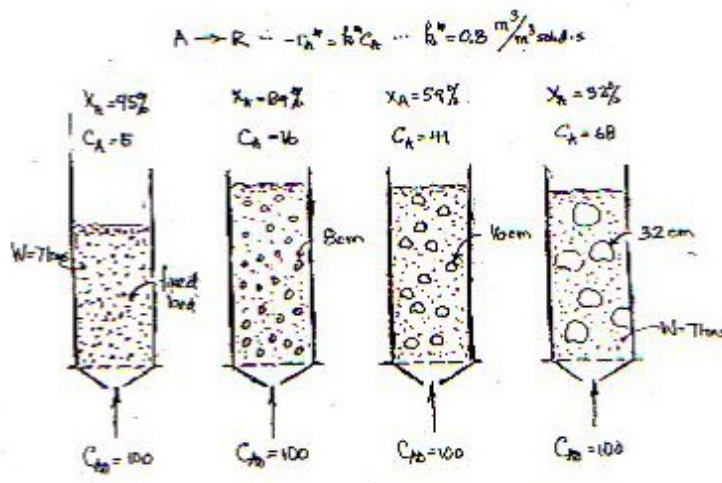


Figure 15.

Next, for reactions in series with the intermediate as the desired product, we see the results shown in Fig. 16

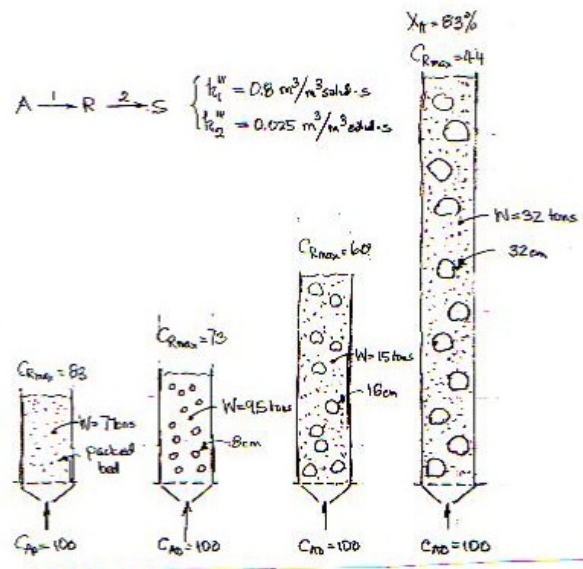


Figure 16.

Finally tall narrow beds behave better than fat shallow beds. Also adding inerts improves bed behavior when all else is kept unchanged - bubble size, volumetric feed rate and amount of catalyst. This is the expected progression with bubble size.

Consequences

All the above findings of this model show that when the rate-controlling step of the process is the chemical reaction step then the behavior of the reactor is strongly affected by the bubble size in the bed, presence of inerts mixed with the catalyst solids, and bed geometry. This is shown in Fig.17 and this is quite different from packed bed behavior.

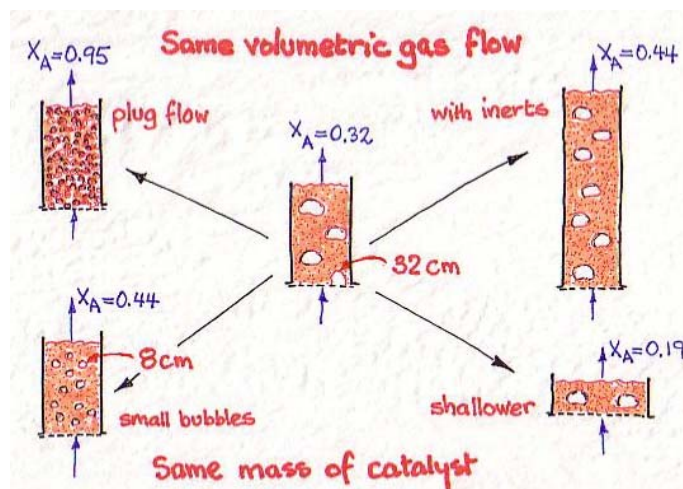


Figure 17.

So let me ask - if you want to develop a model for a reaction controlled BFB reactor

- * Have you tried to extrapolate its predictions to different bubble sizes?
- * Is bubble size a primary variable in your model?
- * Have you accounted for the presence or absence of inerts, as well as for bed geometry?

If your answer is “no” to the above questions then what you are proposing is not an engineering model, which cannot reliably predict reactor behavior.

Problems with Prediction and Scale Up

First, from a laboratory unit it is difficult to tell what will be the bubble size in a scaled up reactor because so many factors will affect it - type of distributor, changing fraction of fines generated during reaction, coalescence of bubbles as they rise in the bed, etc. Also it is hard to get a reasonable estimate of the size of the crazily changing shapes of the bubbles.

Thus scale up and design is fraught with uncertainty. Maybe one should build a cold (hydrodynamic) model. Certainly one should learn from previous experience, or as our friendly bridge player would say

“one peek is worth two finesses”

To conclude, when the chemical step of a reaction process is rate controlling then BFB reactor models will likely give unreliable prediction of reactor behavior, such as shown in Figure 17. In these situations it is probably better to look for a different type of reactor, not a BFB.

On the other hand, the BFB is certainly useful for systems when heating effects are rate-controlling, such as in highly exothermic or endothermic reactions, or where temperature effects dominate.

References.

1. H.F, Johnstone and coworkers, *AICHE Journal*, 1, 318, 349 (1955).
2. J.F. Davidson and D. Harrison, *Fluidized Particles*, Cambridge University Press, New York, 1963.
3. D. Kunii and O. Levenspiel, *Ind. Eng. Chem., Process Design and Development*, 7, 481 (1968).
4. O. Levenspiel, *Chemical Reaction Engineering*, Third ed., Chap. 20, Wiley, New York.