can. This difference along with most of the significant differences between the voids and bubbles stems from the fact that voids have no surface tension effects associated with them. This means that solids are free to fall through the voids. This often occurs and is one of the principle mechanisms accounting for the spontaneous break up of voids. (Davidson and Harrison, 1982) In addition, the gas in the voids is not confined there. It can flow out into the emulsion and the gas in the emulsion phase can flow into the bubbles. The gas in the voids has been found to exhibit the flow pattern shown in Figure 9. (Davidson and Harrison, 1982) This circulation allows for greater gas-solids contacting which in turn increases the amount of heat and mass that can be transferred from one phase to the other. The importance of the region of the emulsion immediately surrounding each bubble where most of the mixing occurs has led some researchers to suggest that this region be considered a third phase called the cloud phase. (Peters et al., 1982)

The gas circulation has the additional effect of pulling solid particles into a wake region behind each void as is shown in Figure 10. The solids in the wake are pulled along with void as it rises through the bed. Since the solids can not accumulate at the top of the bed there must be a net downward flow of solids in the emulsion

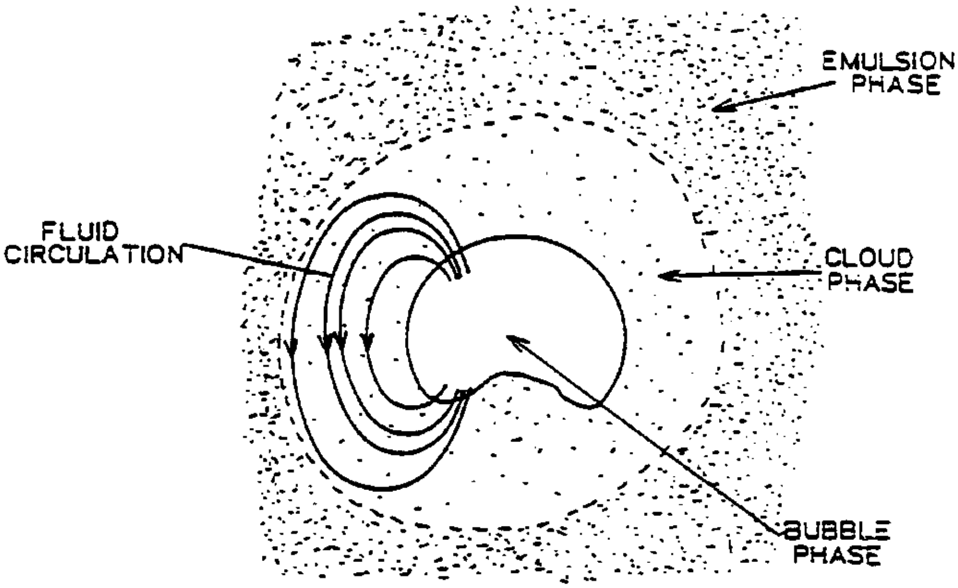

Figure 9. The gas flow pattern in the vicinity of a void.

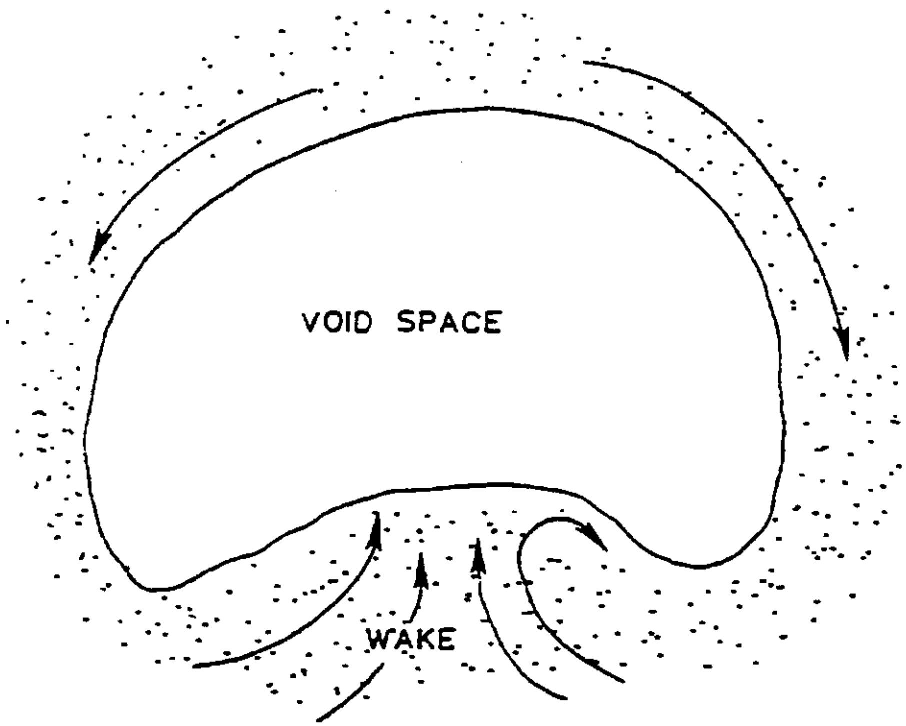

Figure 10. The pattern of solids movement in the vicinity of a void.

phase. The large scale mixing of solids in fluidized beds stems from this circulation pattern. The solids circulation is also responsible for the reverse flow of gas in the emulsion phase that is encountered at high gas flow rates. The rate of solids circulation in the bed increases as the flow rate of the gas increases. Eventually the particles are falling at a sufficient rate for their drag to reverse the flow of the gas in the emulsion. The back flow of the emulsion gas can have a significant effect on the concentration profiles encountered in a fluidized bed reactor. (Fryer and Potter, 1972)

When the bubbles reach the top of the reactor they burst through the surface of the bed spraying solids up into the freeboard area above the bed. The bed's surface is constantly fluctuating up and down as bubbles break through. The gas enters the freeboard after leaving the bed. Here the majority of the solids entrained in the gas by the bursting voids disengage from the flow and return to the bed. (Cheremisinoff and Cheremisinoff, 1984) Figure 11 is a diagram of all the regions present in a fluidized bed.

Previous Modeling. As can be imagined when considering the wide spread use of fluidized beds there has been a large number of attempts to model them. The complexity of the phenomena occurring in fluidized beds

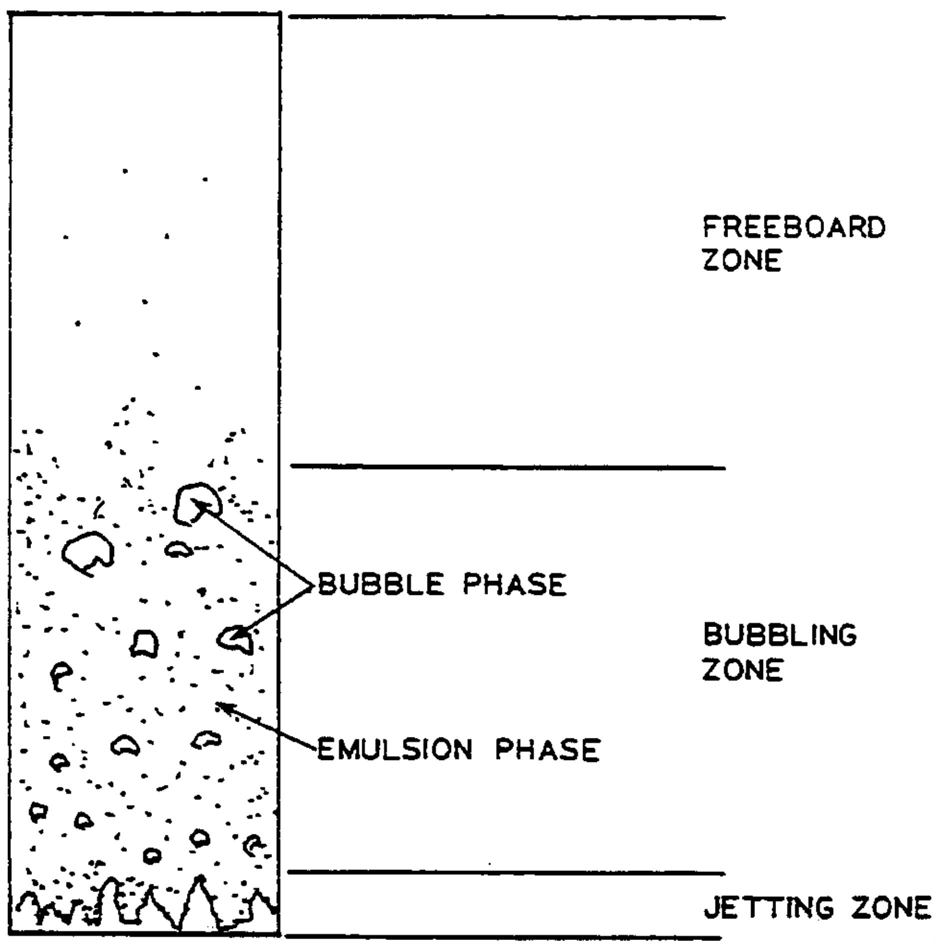

Figure 11. The different regions typically found in fluidized beds.

insures that there are nearly as many different approaches to modeling the reactors as there have been attempts to do so. The models are most effectively categorized based on the extent to which they simplify the behavior of the reactors. In modeling fluidized beds it is necessary to consider phenomena occurring on two different scales. The first scale involves those phenomena that occur over the entire bed. Considerations on this scale include such items as the number of phases considered, the number of different regions considered, the type of flow present in each phase or region, and the size of each region. The other scale relates to the phenomena occurring around each bubble. Considerations associated with this scale include such items as mass transfer, heat transfer, and reaction rates. Generally the small scale considerations supply parameters to be used in the models built based on the large scale considerations.

The simplest approach to modeling a fluidized bed reactor is to assume that the reactor can be approximated by a single ideal reactor. The well mixed tank reactor is the most obvious choice. The fluidized bed can be seen to be violently mixing at all times making the well mixed reactor seem to be a good choice. This model is often used to model the heat transfer characteristics of a fluidized bed. (Kunii and Levenspiel, 1977) Figure 12 is a schematic diagram of a well mixed model of a fluidized bed reactor. The equations for this type of ideal reactor come directly from the standard treatments of well mixed reactors. The equations contain only one term that is based on the characteristics of a given bed. Thus it can be seen that this model of a fluidized bed would be very easy to use. Only one parameter requires any detailed analysis of the bed. Extensive treatments of the equations can be found in many sources. (Chen, 1983, Froment and Bischoff, 1979) Scale-up using this model would be relatively easy.

However, in many cases this model does not give acceptable results. (Davidson and Harrison, 1982) Close examination of a fluidized bed shows that a well mixed model is actually only accounting for the solid material. Since the solids usually have a much higher heat capacity than the gas, the model is useful in modeling the thermal properties of the bed. On the other hand, the gases in the reactor are often intimately involved in the reaction taking place. The well mixed model is accordingly less accurate in predicting conversions in the reactor. (Zabrodsky, 1963)

Tracer studies indicate that the behavior of the gases in the reactor can be approximated by assuming that the reactor is a plug flow reactor. (Yates, 1983) This assumption is essentially presuming that the bubbles rise

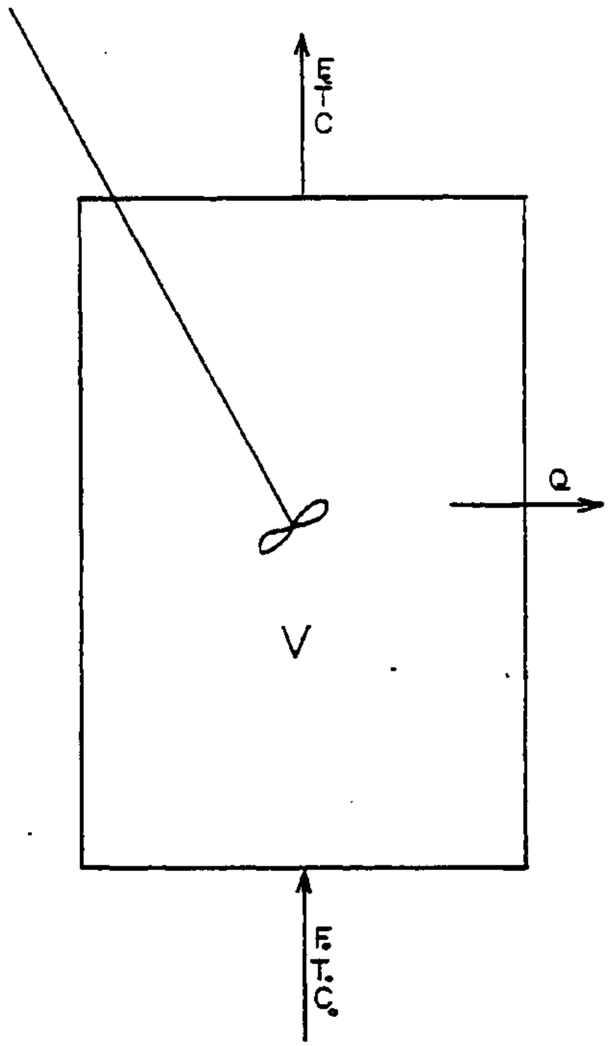

Figure 12. The well mixed reactor model.

quickly though the bed, carry most of the gas flow, and have only minor interaction with the solids.

Once again standard equations can be used. The availability of these extensive analysises is one of the primary motivations in trying to use simple idealized reactor approximations. The use of the appropriate equations requires a knowledge of the heat transfer coefficient. This coefficient is determined from the small scale model used to describe the reactor. The plug flow model ignores the presence of the solid particles. It is effective when used on reactors in which the solids serve only as a heat transfer medium or play no role at all. Obviously the usefulness of this model is limited.

The next level of sophistication involves accounting for both of the two phases that are present in aggregate fluidized beds. In modeling this two phase system, separate reactor types can be posed for each phase. The simplest combination of reactors that is appropriate is a well mixed reactor linked to a plug flow reactor. The well mixed reactor will describe the behavior of the emulsion phase and the plug flow reactor will describe the behavior of the bubble phase. In this type of model, the ideal reactor equations would be modified to allow for transfer from one phase to the next. This model requires the derivation of an expression for the mass and heat transfer coefficients between the bubble phase and the emulsion phase and an expression for the volume of the bed each phase occupies. The volumes are relatively easy to obtain using the fact that any flow above the minimum required for fluidization is in the bubble phase. The transfer rates are more complex and depend on the small scale model used.

A more accurate model would take into account the fact that while the solid particles behavior closely resembles ideal mixing the behavior of the gas in the emulsion phase does not. (Froment and Bischoff, 1979) The gas in the emulsion phase would be better approximated using a flow model with effective dispersion. The effective dispersion coefficient must then be determined. The only practical way to obtain this number that has been found so far is by experiment. Using tracer studies and residence time distributions it is possible to arrive at a reasonably good value for the coefficient. The main drawback to this approach is that not only is the model non-predictive, it can not be applied accurately to different reactors.

These models, while more accurate than the single ideal reactor models, still are not sufficient for some modeling requirements. The next improvement that has been introduced is to use multiple reactors for each phase. The simplest of these multiple reactor models is the tanks in series model. This model postulates that the emulsion phase can be better represented by a series of well stirred tanks in series. It retains the plug flow model for the bubble phase. This model is similar to the dispersion model with the determination of the dispersion coefficient replaced by a determination of the number of stirred tanks required to represent the phase.

All the models up to this point have only dealt with the main region of fluidized beds. They have not dealt specifically with any of the other regions. The next level of complexity is include specific provisions for these areas in the model. Figure 13(a) shows one typical method of dealing with the jetting region. Another area of interest is the freeboard region above the bed. Here there is no emulsion phase, however, there are some small particles still suspended in the gas stream. In addition, the lack of most of the solids has a major affect on the velocity of the gas. A combination model that will account for this region is shown in Figure 13(b). Some models attempt to break both the emulsion phase and the bubble phase into several ideal reactors as is shown in Figure 13(c). It is possible to create a practically unlimited number of such combination models. These models are considerably more accurate than the simpler models but require much more

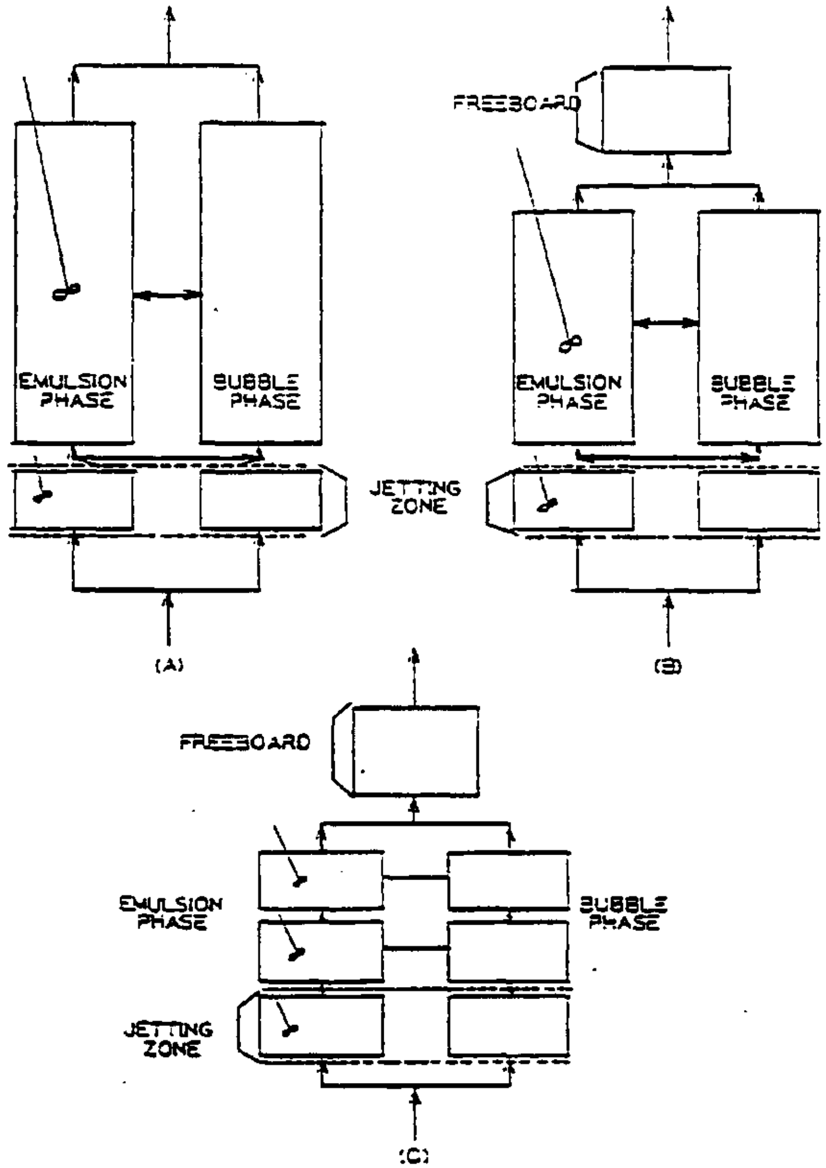

Figure 13. Three multiple reactor models.

work to develop. In addition, there are many cases where even these combination models are insufficient.

The highest level of sophistication found in the modeling of fluidized beds involves the use of non-ideal reactors. These models sacrifice the mass of work that has been done on the ideal reactors for improved accuracy and a better physical representation of the bed. There are three principle models of this type. They are the bubbling bed model of Kunii and Levenspiel (1977), the counter current backmixing model of Stephens, Sinclair, and Potter (1972), and the bubble assemblege model of Kato and Wen. (1969) Many workers have taken the basic ideas presented in these non-ideal reactor models and modified them slightly to account for details that the original authors neglected for simplicity.

Some other approaches that have been examined are residence time distributions and stochastic modeling. (Orcutt et al.,1982, Too et al., 1983) However, neither area has received the extensive treatments that the more traditional modeling approaches have.

The bubble assemblege model was chosen for use in the research effort. The bubble assemblege model is accurate and can describe the behavior of many different types for fluidized beds. In addition, it makes use of algebraic equations only. No differential equations must be solved in conjunction with this model.

The small scale phenomena associated with fluidized beds are nearly always modeled empirically. There are many compilations of these correlations. (Too et al., 1983, Viswanathan, 1982) There has, however, been some work on a fundamental level in conjunction with these phenomena. The first step in developing a small scale model is to make some assumption about the shape of the bubbles. Observations of bubbles bursting through the surface of a fluidized bed show that at least the caps of the bubbles are spherical. X-ray pictures of operating beds show that the spherical bubble caps are maintained well within the bed. (Davidson and Harrison, 1982) The most widely used assumption of the bubble's shape, based on this observation, is that a bubble is spherical. This assumption makes calculations involving the bubble's volume and surface area relatively simple. The errors caused by assuming spherical bubbles are usually assumed to be negligible compared to the other assumptions needed to model a fluidized bed.

The gas circulation pattern around each bubble that was described earlier has also been subjected to simplifying assumptions. There are generally three levels of simplification of the flow pattern that are commonly used. These levels are shown in Figure 14.

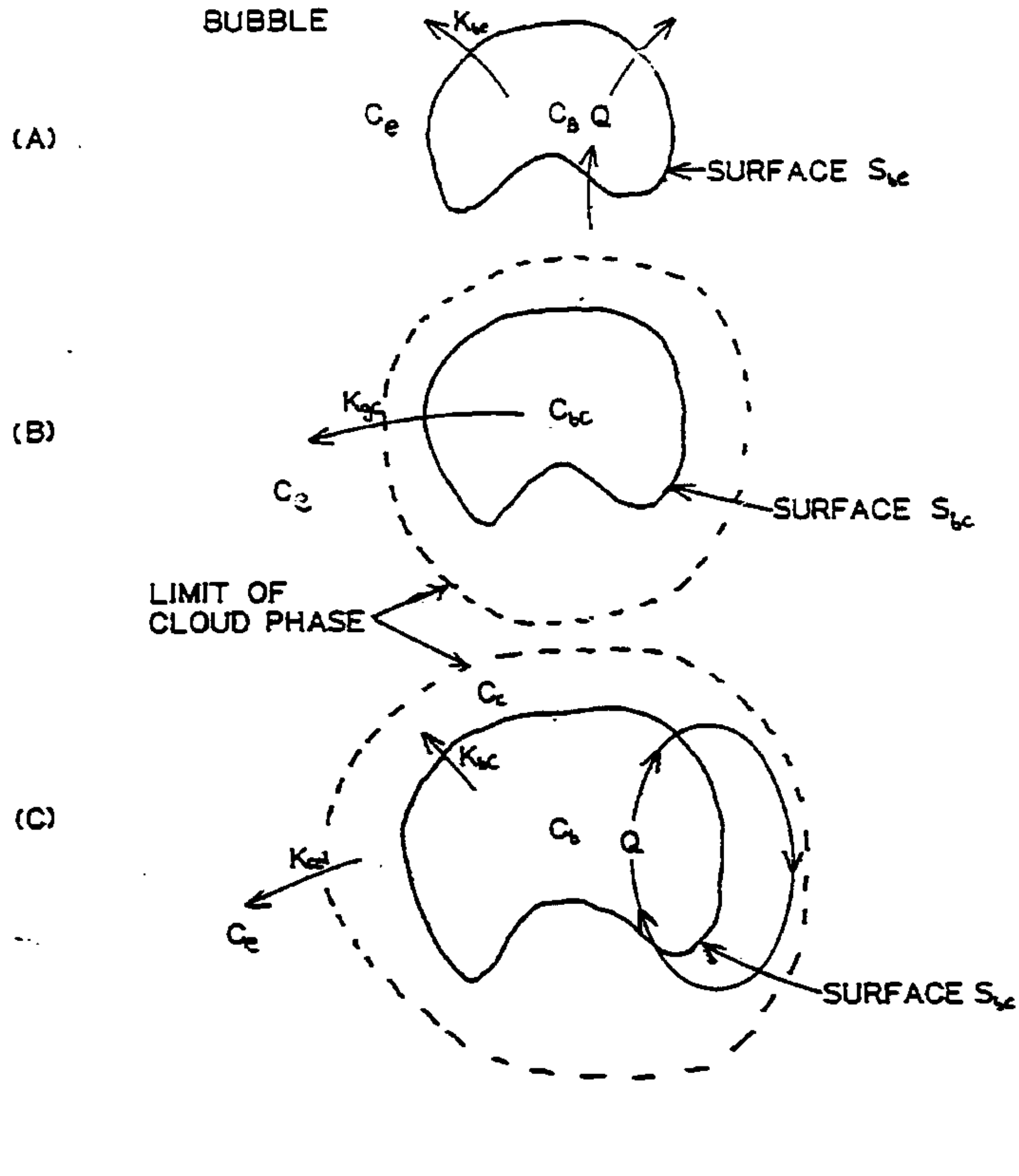

Figure 14. Three models used to represent the gas flow near a void. A. Davidson B. Partridge and Rowe C. Kunii and Levenspiel.

In the first approach, Figure 14(a), the presence of the return flow is ignored. Using this approach, the transport of material from the bubble to the emulsion can be seen as stemming from two sources - the bulk flow from the bubble and diffusion. Assuming these processes are additive one gets :

$$\frac{d\ (V_b C_b)}{dt} = q + k_{be} S_{be} (\ C_b - C_e\ ) \qquad (1)$$

so the overall rate is :

$$K_{bc} = (\ q + k_{be} S_{be}) / V_b \qquad (2)$$

At this point some assumptions would have to be made or some correlation used to get expressions for q and k_{be}. Davidson derived an expression for q that is deceptively simple. (Davidison and Harrison, 1982)

$$q = (\frac{3}{4})\pi U_{mf} d_p^2 \qquad (3)$$

k_{be} is arrived at by analogy to diffusion from a spherical-cap shaped gas bubble in a liquid using boundary layer analysis. (Yates, 1983)

$$k_{be} = 0.975\ D_g^{0.5}\ d_p^{-0.25} g^{0.25} \qquad (4)$$

The second approach, shown in Figure 14(b), assumes that the cloud to emulsion transfer rate will be the most important. This transfer will occur mainly by diffusion so

$$\frac{d\ (\ V_{bc} C_{bc})}{dt} = k_{gc} S_{bc} (\ C_{bc} - C_e) \qquad (5)$$

In this case, the transfer rate was estimated by Partridge and Rowe by analogy to the transfer from a drop of one immiscible liquid rising in another. (Yates, 1983) The Sherwood number for this process has been correlated as

$$Sh_c = k_{gc} d_c / D_g = 2 + 0.69\ Sc^{1/3} Re_c^{1/2} \qquad (6)$$

where $Sc = \mu_f / \rho D$ and Re_c is defined in terms of the relative velocity between the rising cloud and the emulsion. The rate of transfer per unit volume of cloud space can then be arrived at

$$K_{b\ ce} = k_{gc} \pi d_c^2 \in / V_{bc} = 3.9 \quad D_c Sh_c / V_{bc}^{2/3} \qquad (7)$$

The third approach, shown in Figure 14(c), assumes that both the rate of transfer to the cloud phase and to the emulsion phase are important. This was the approach of Kunii and Levenspiel. (1977) The coefficient for the the transfer between the bubble and the cloud was taken to be the same as that derived by Davidson for the transfer from the bubble to the emulsion. The cloud to emulsion coefficient was obtained from Higbie penetration theory. (Kunii and Levenspiel, 1977) The expression for this last coefficient is :

$$k_{ce} = 6.78 \left(\epsilon_{mf} D_g U_b / d_b^3 \right)^{1/2} \qquad (8)$$

The overall rate was then taken to be

$$1/k_{be} = 1/k_{bc} + 1/k_{ce} \qquad (9)$$

It has been found that for most practical systems $K_{be} = K_{ce}$. This gives a result very similar to the obtained by using the second approach.

All the expressions that were derived for the mass transfer coefficient only considered a single isolated bubble. Grace and Harrison found that when bubbles are close to one another the rate of transfer from each is considerably greater than it would be if the bubbles were isolated. (Grace and Madsen, 1980) Sit and Grace (1981) conducted a comparison of these values and suggest that the coefficients obtained from isolated bubble models be multiplied by 1.32. This number is derived on the basis that there is about 1.8 times better transfer from bubbles that interact and approximately 40 % of the bubbles in the bed are interacting.

For heat transfer, only considering the interactions between the bubbles and the emulsion is not sufficient. The interaction of each phase with the wall of the vessel is also important. In fact, most researchers have found that the interactions involving the wall are the most important interactions with respect to heat transfer.

Much of the heat transfer work done with respect to fluidized beds has focused on obtaining empirical equations that relate the dimensionless quantities identified by dimensional analysis to one another. (Kunii and Levespiel, 1977) While some of these equations are fairly successful they do not provide much basic information about the processes occurring in the fluidized bed. The heat transferred from the walls of a fluidized bed is much greater than that that would be transferred through the wall if the reactor contained a fixed bed. There have been three main approaches to explaining why this is so.

Levenspiel explained this by assuming the particles falling along the wall of the reactor scour away the boundary layer. If one then assumes that the fluid flow near the wall is laminar an expression can be derived that agrees with some of the data obtained from fluidized beds. (Kunii and Levespiel, 1977)

A second approach that has been used to explain the enhanced heat transfer capabilities of fluidized beds is to consider packets of hot solid particles impacting the wall and clinging there for a short period of time before being replaced by a fresh packet. This type of model was developed by Mickley and Fairbanks. (Kunii and Levespiel, 1977) They also assumed that the portion of the wall covered by bubbles does not contribute significantly to the heat transfer capabilities of the bed. By properly adjusting the parameters one can obtain a better fit to the data than Levenspiel's model.

The final approach commonly used is to consider the portion of the surface covered by the bubbles that was neglected by Mickley. Wicke and Fetting have done some of the most recent work in this area. (Kunii and Levespiel, 1977) They found that their model was able to account for the affects changes in the gas velocity had more accurately than the other models.

All of these models require some degree of empirical fitting. Once the values of the empirical parameters are obtained, however, the models are theoretically able to predict the heat transfer characteristics of any bed.