is tuned for set point response, the same setting gives very poor load response, and vice versa.

The response of the proposed algorithm does not deteriorate when errors are present in the process parameters. Furthermore, only one algorithm is needed to compensate for both set point and load changes. This is a distinct advantage over the previously reported minimal algorithms and discrete P.I. algorithms. Since the proposed algorithm views deviations in the output of the process from the set point value as an equivalent step disturbance in the input, the response is always stable.


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### NOTATION

$a$ = constant used to define dead time
$G_p(s)$ = process transfer function
$K_p, K_c$ = process gain, controller gain
$m$ = manipulated variable
$T$ = sampling period
$X^*$ = input to the process
$y$ = output of the process

#### Greek Letters

$\alpha$ = constant defined in Equation (2)
$\beta$ = constant defined by Equation (9)
$\epsilon_\tau$ = deviation in process parameter, $\tau$
$\epsilon_k$ = deviation in process parameter, $K_p$
$\lambda$ = fraction used to define time delay
$\tau, \tau_I$ = process time constant, integral time

#### Subscripts

$a$ = algorithm
$p$ = process
$i$ = value of the variable between the time $iT$ and $(i + 1)T$

#### Superscripts

set = set point of the variable
$*$ = variable evaluated $\lambda T$ time later

### LITERATURE CITED


Luyben, W. L., "Damping Coefficient Design Charts for Sampled-Data Control of Processes with Deadtime," *AIChE J.*, **18**, No. 5, 1048 (1972).

Mosler, H. A., L. B. Koppel, and D. R. Coughanowr, "Process Control by Digital Compensation," *ibid.*, 768 (1967).

Shunta, J. P., and W. L. Luyben, "Studies of Sampled-Data Control of Distillation Columns. Feedback Control of Bottoms Composition with Inverse Response Behavior," *Ind. Eng. Chem. Fundamentals*, **10**, No. 3, 486 (1971).

Ziegler, J. C., and N. B. Nichols, "Optimum Settings for Automatic Controllers," *Trans. Am. Soc. Mech. Engrs.*, **64**, 759 (1942).



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# Reaction Near the Grid in Fluidized Beds


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There is growing recognition that two-phase models for fluidized-bed reactors should take account of end effects. Experimental results show that bubbling-bed models do not properly represent reaction near the gas distributor (Chavarie and Grace, 1975) or in the freeboard region (Furusaki et al., 1976). In this note we consider reaction in the vicinity of the grid.

### EARLIER MODEL

Behie and Kehoe (1973) proposed a two-phase model which extends one of the well-known Orcutt models (Orcutt et al., 1962) by treating a plug flow, jet region devoid of particles in series with the bubble phase. Gas in the entire dense phase is assumed to be perfectly mixed. Since the resistance to mass transfer between grid jets and the dense phase is much lower (Behie, 1972) than that between bubbles and the dense phase, the grid model predicts significantly higher conversions than the corresponding Orcutt model, providing that the kinetic rate constant is sufficiently large for the rate of reaction to be controlled by hydrodynamic factors.

The case considered by Behie and Kehoe involves a first-order, constant volume, gas phase reaction $A \rightarrow B$ catalyzed by the solid particles. Temperature gradients are neglected. The flow patterns assumed for the three phases are shown schematically in Figure 1. Note that the entire flow of gas $UA$ is assumed to pass through the jets and then to divide itself between the bubble phase and dense phase at the top of the jets. The mass balance equations for the three phases are

Jet phase $(0 \leq x \leq h)$:

$$U\frac{dC_j}{dx} + k_j a_j (C_j - C_d) = 0 \quad (1)$$

Bubble phase $(h < x \leq H)$:

$$\beta U \frac{dC_b}{dx} + k_b a_b (C_b - C_d) = 0 \quad (2)$$

Dense phase $(0 \leq x \leq H)$:

$$U(1-\beta)(C_d - C_{jh}) + \int_0^h k_j a_j (C_d - C_j)\,dx + \int_h^H k_b a_b (C_d - C_b)\,dx + k_r C_d H_{mf} = 0 \quad (3)$$


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where $\beta$ is the fraction of the incoming gas entering the bubble phase (assumed to be independent of height), and $k_j a_j$ and $k_b a_b$ are the interphase mass transfer coefficient $\times$ interfacial area/unit bed volume products for the jet and bubble regions, respectively. Equations (1) and (2) can be integrated readily to express $C_j$ and $C_b$ explicitly in terms of $C_d$. $C_d$ is then found from Equation (3), and the exit concentration for the reactor is obtained from a mass balance; that is

$$C_{Ae} = \beta C_{bH} + (1 - \beta) C_d \tag{4}$$

This yields

$$\frac{C_{Ae}}{C_{Ao}} = \frac{1 + \beta(K-1)e^{-(m_j+m_b)}}{1 + K - \beta e^{-(m_j+m_b)}} \tag{5}$$

where

$$K = \frac{k_r H_{mf}}{U} \tag{6}$$

is a dimensionless rate constant, and

$$m_j = \frac{k_j a_j h}{U}; \quad m_b = \frac{k_b a_b (H-h)}{\beta U} \tag{7}$$

are dimensionless mass transfer parameters for the jet region and bubble region, respectively. Predictions for the two cases used as illustrative examples by Behie and Kehoe are shown in Figure 1.

## EXTENDED GRID MODELS

Two key assumptions of the Behie and Kehoe model are that the gas in the dense phase is perfectly mixed and that there are no particles dispersed in the jet phase. Backmixing of gas in the bubbling region is caused by adsorption and desorption processes and by drag due to solid particles moving downwards to compensate for upward transport of solids in bubble wakes (Latham and Potter, 1970). Merry (1976) has shown that some entrainment of solids does occur into grid jets. While the resulting solids flow pattern modifies the streamlines for the fluidizing fluid, massive solids backflow and gas backmixing appear unlikely, although local gas downflow can occur for the analogous case of spouted beds (van Velzen et al., 1974).

In order to observe the sensitivity of modeling to the assumptions of perfect gas phase mixing in the dense phase and no solids in the jets, we consider two simple alternate models, illustrated schematically in Figure 1. Both models lead to analytic solutions for first-order reactions. In the first, the entire dense phase is treated as a stagnant region (no vertical gas flow as in the bubbling-bed model of Kunii and Levenspiel, 1969). The entire gas flow passes through the jet and bubble phases, both of which are assumed to be in plug flow. Different interphase mass transfer rates are again assumed between the dense phase and the jet and bubble phases. Some solids are assumed to be dispersed in the jet phase, with the volumetric concentration of particles there being $\sigma$.

The mass balance for reactant $A$ in the bubble phase is identical to Equation (2), but with $\beta = 1$. For the other phases, the new equations are:

Jet phase ($0 \leq x \leq h$):

$$U\frac{dC_j}{dx} + k_j a_j (C_j - C_d) + \frac{k_r \epsilon_j \sigma C_j}{(1 - \epsilon_{mf})} = 0 \tag{8}$$

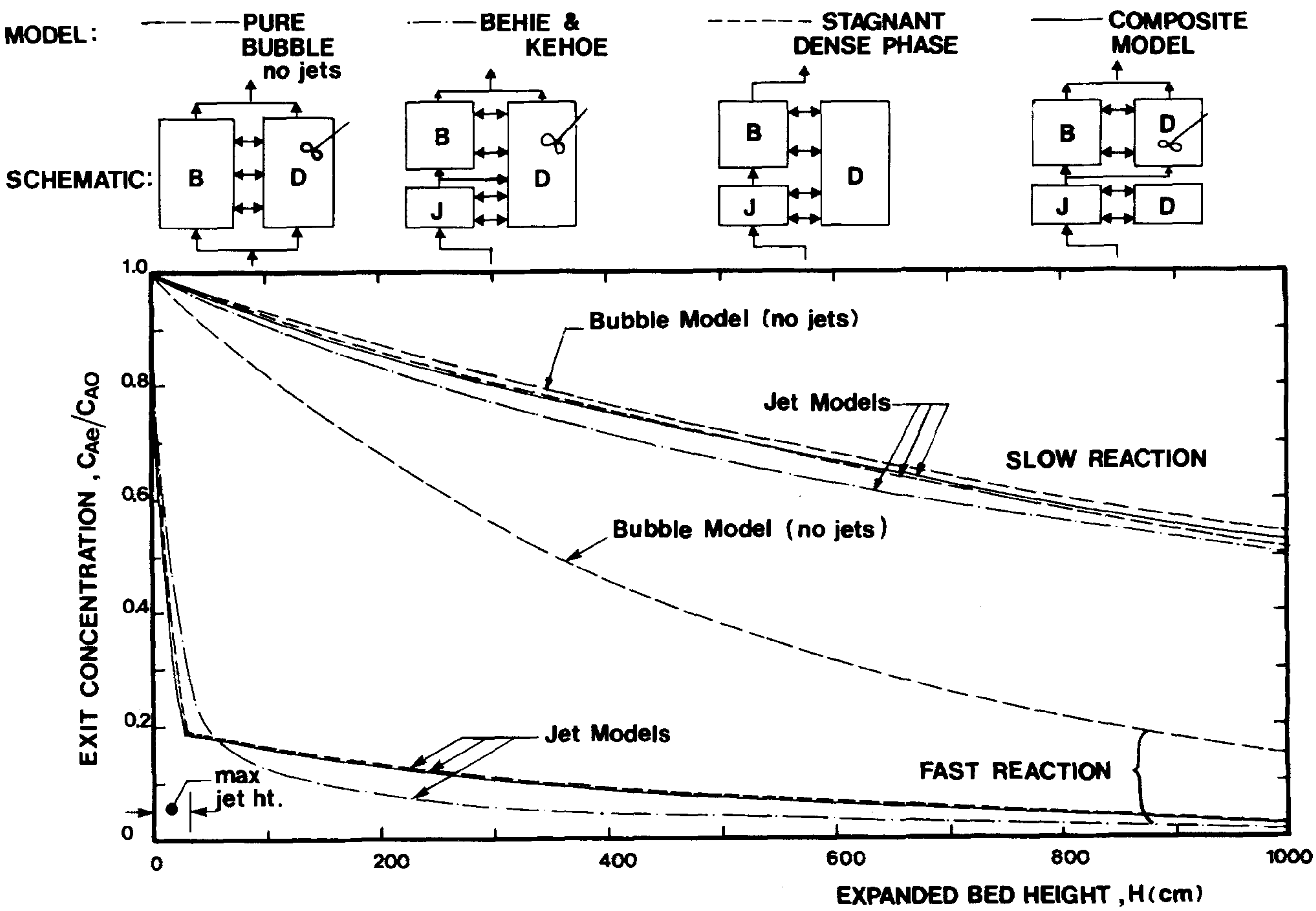


Fig. 1. Predictions of three fluidized-bed reactor models including the grid jet region compared with a bubbling bed model (Orcutt et al., 1962) in which bubbles are assumed to form right at the distributor. Conditions are the same as in the illustrative example of Behie and Kehoe (1973).

Dense phase ($0 \leq x \leq h$):

$$k_j a_j (C_j - C_d) = k_r(1 - \epsilon_j) C_d \qquad (9)$$

Dense phase ($h < x \leq H$):

$$k_b a_b (C_b - C_d) = k_r(1 - \epsilon_b) C_d \qquad (10)$$

The exit concentration is simply $C_{bH}$. Solving these equations, we obtain

$$\frac{C_{Ae}}{C_{Ao}} = \exp\left\{ - \frac{m_j K_j}{m_j + K_j} - \frac{K_j \epsilon_j \sigma}{(1 - \epsilon_j)(1 - \epsilon_{mf})} - \frac{m_b K_b}{m_b + K_b} \right\} \qquad (11)$$

where $m_b$ and $m_j$ are as defined in Equation (7), only with $\beta = 1$, while

$$K_j = \frac{k_r(1 - \epsilon_j) h}{U}; \quad K_b = \frac{k_r(1 - \epsilon_b)(H - h)}{U} \qquad (12)$$

The three terms in Equation (11) arise from reaction, respectively, in the lower dense phase ($x \leq h$), in the jets themselves, and in the upper ($x > h$) dense phase level with the bubbling region.

For the other alternate model, labeled composite model in Figure 1, the dense phase is considered to be composed of two parts. In the lower, from the grid to the top of the grid jets, gas is assumed to be stagnant as in the previous case. At the top of the jets, gas is assumed to distribute itself, a fraction $\beta$ passing in plug flow through a solids free bubble phase and the remainder perfectly mixed in an upper dense phase region. Mass balances may now be written as for the corresponding cases above. The resulting exit concentration is

$$\frac{C_{Ae}}{C_{Ao}} = \left[ \frac{1 + \beta(K_b - 1) e^{-m_b}}{1 + K_b - \beta e^{-m_b}} \right] \times \exp\left\{ - \frac{m_j K_j}{m_j + K_j} - \frac{K_j \epsilon_j \sigma}{(1 - \epsilon_j)(1 - \epsilon_{mf})} \right\} \qquad (13)$$

where $\beta \approx 1 - U_{mf}/U$ from the two-phase theory of fluidization.

## COMPARISON OF MODELS

Exit concentrations are shown in Figure 1 as a function of total bed height $H$ for each of the models discussed above using the physical properties defined in their Table 1 by Behie and Kehoe (1973) with 0.0127 m diam orifices, $h = 0.305$ m, and kinetic rate constants differing by a factor of 100. The fluidizing gas was assumed to have a density of 1.2 kg/m$^3$.

The basic qualitative conclusion of Behie and Kehoe is valid regardless of which grid model is adopted; that is, ignoring the jet region causes little error for a slow (kinetics controlled) reaction, whereas there is a very marked influence of the grid region for fast reactions unless the bed is very deep. Quantitatively, both alternate models generally predict less conversion than the Behie and Kehoe model which, as shown by Errazu and de Lasa (1977), inevitably approaches the predictions for a single-stage, continuous, stirred tank reactor when $m_j >> 1$. The curves plotted in Figure 1 are for $\sigma = 0$. Experiments indicate $\sigma$ lies in the range 0.001 to 0.006 (Merry, 1976). For the conditions used by Behie and Kehoe, reaction due to solids entrained in the jets has negligible influence on the overall conversion for this range of $\sigma$ but could become important for fast reactions, especially for lower $m_j$ and high heats of reaction.

There is a need for further work on the grid region. In particular, more jet to dense phase transfer rates must be measured to allow generalizations of the results of Behie (1972). Since the grid region is commonly a region of marked temperature gradients, energy balances must also be considered when we apply the grid models for many reactions of practical importance.

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## NOTATION

$A$ = cross-sectional area of bed
$a_b$, $a_j$ = interfacial area of bubble, jet phase per unit bed volume
$C_{Ae}$, $C_{Ao}$ = exit, initial concentration of reactant $A$
$C_b$, $C_d$, $C_j$ = bubble phase, dense phase, jet phase concentration of $A$
$C_{bH}$, $C_{jh}$ = value of $C_b$ at $x = H$, value of $C_j$ at $x = h$
$H$, $H_{mf}$ = total bed height, height at minimum fluidization
$h$ = jet height
$K$, $K_b$, $K_j$ = dimensionless rate constants defined by Equations (6) and (12)
$k_b$, $k_j$ = bubble, jet to dense phase mass transfer coefficient
$k_r$ = first-order kinetic rate constant based on unit volume of dense phase
$m_b$, $m_j$ = dimensionless mass transfer parameters defined by Equation (7)
$U$, $U_{mf}$ = superficial gas velocity, minimum fluidization velocity
$x$ = distance above the grid
$\beta$ = fraction of gas flow in the bubble or jet phase
$\epsilon_b$, $\epsilon_j$ = fraction of cross-sectional area occupied by bubble, jet phase
$\epsilon_{mf}$ = bed voidage at minimum fluidization = dense phase voidage
$\sigma$ = fraction of jet volume occupied by particles

## LITERATURE CITED

Behie, L. A., "Momentum, Heat and Mass Transfer from a Grid Jet in a Large Gas Fluidized Bed," Ph.D. dissertation, Univ. Western Ontario, Canada (1972).

———, and P. Kehoe, "The Grid Region in a Fluidized Bed Reactor," *AIChE J.*, **19**, 1070 (1973).

Chavarie, C., and J. R. Grace, "Performance Analysis of a Fluidized Bed Reactor, II. Observed reactor behaviour compared with simple two-phase models," *Ind. Eng. Chem. Fundamentals,* **14**, 79 (1975).

Errazu, A. F., and H. I. de Lasa, "A Fluidized Bed Catalytic Cracking Regenerator Model: Grid Effects," 27th Canadian Chem. Eng. Conf., Calgary, Canada (1977).

Furusaki, S., T. Kikuchi, and T. Miyauchi, "Axial Distribution of Reactivity inside a Fluid Bed Contactor," *AIChE J.*, **22**, 354 (1976).

Kunii, D., and O. Levenspiel, *Fluidization Engineering*, Wiley, New York (1969).

Latham, R., and O. E. Potter, "Back-mixing of Gas in a 6-inch Diameter Fluidized Bed," *Chem. Eng. J.*, **1**, 152 (1970).

Merry, J. M. D., "Fluid and Particle Entrainment into Vertical Jets in Fluidized Beds," *AIChE J.*, **22**, 315 (1976).

Orcutt, J. C., J. F. Davidson, and R. L. Pigford, "Reaction Time Distributions in Fluidized Catalytic Reactors," *Chem. Eng. Progr. Symposium Ser., No. 38,* **58**, 1 (1962).

van Velzen, D., H. J. Flamm, and H. Langenkamp, "Gas Flow Patterns in Spouted Beds," *Can. J. Chem. Eng.*, **52**, 145 (1974).

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