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Effect of Flow Maldistribution on Conversion and Selectivity in Radial Flow Fixed-Bed Reactors

This paper examines the effect of flow maldistribution on the predicted conversion and selectivity in a radial flow fixed-bed reactor. A simple model was developed to relate gas maldistribution to the catalyst bed to the conversion with first- and second-order reactions and to selectivity for first-order reactions in series and parallel. For the cases considered, the conversion debit due to maldistribution of the gas phase was as much as 11%. The model was extended to cover adiabatic conditions for simple first-order reactions. For an exothermic reaction, maldistributions can enhance conversion over that obtained with a uniformly distributed gas phase.

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SCOPE

An advantage of radial flow fixed-bed reactors over axial flow units is the high flow surface area per volume of catalyst. This results in narrow, low pressure drop beds. Radial reactors with these low pressure drop configurations can be subject to uneven gas distribution along the axial length.

Fluid dynamic models of the gas distribution were developed by Dil'man et al. (1971) and Genkin et al. (1973) and extended by Kaye (1978). Lamba and Dudukovic (1975) investigated the effect of radial dispersion by the catalyst bed on conversion. The consequences of maldistributed gas flow to the catalyst bed has not been studied and is a concern in the design of low pressure drop, radial reactors. The objective of this study was, therefore, to assess the magnitude of the effects of maldistribution on reactor operation.

A derivation is presented of a simple model which relates inlet flow distribution to conversion and selectivity. The model assumes that the gas moves radially in plug flow fashion through parallel elements of the catalyst bed without axial flow by either convection or dispersion and without radial dispersion. Both isothermal and adiabatic operation are considered. For the purpose of this study, the axial velocity profiles were approximated by a simple power law expression.

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CONCLUSIONS AND SIGNIFICANCE

For the particular case of isothermal flow from the central pipe outward, analytical expressions were developed which relate the conversion to the degree of maldistribution for simple first- and second-order reactions and the selectivity to the maldistribution for series and parallel reactions. Examples of these effects are given for selected degrees of maldistribution. For the cases considered, the conversion debit could be as much as 11%.

The effect of maldistribution with a first-order reaction under adiabatic conditions was also developed. The effects, however, must be determined numerically. It was found that for low conversion in exothermic systems, maldistributions can enhance conversions over those obtained with a uniformly distributed gas phase. This enhancement is attributed to the higher temperature utilization of some sections of the catalyst bed. The magnitude of the maldistribution effects are a maximum with the simple model because of the neglect of axial convection and dispersion, but similar trends may be possible in commercial fixed-bed radial reactors. A more accurate analysis of flow maldistribution would require the solution of the heat and mass balance equations, taking dispersion and axial gas flow into account.

The cases developed in this paper assumed simple kinetic expressions, no initial conversion, no change in the number of moles, and flow from the central pipe outward. The analyses could be extended to more complicated systems without these restrictions and to radial flow from the outer annulus inward.

Radial flow fixed-bed reactors are an attractive alternative to axial flow designs for vapor phase systems. The radial configuration is well suited to operations where a low bed pressure drop is essential or desirable and has found commercial application in catalytic reforming, ammonia synthesis, methanation, and flue gas desulfurization. Low bed pressure drops are possible because of the high external surface area and small bed thickness in the direction of flow. Equivalent bed pressure drops in axial reactors with the same residence time can be achieved only by using large diameter vessels with shallow pancake beds.

Of prime importance in the design of a radial reactor is ensuring a uniform axial distribution of gas to the catalyst bed with a minimum bed pressure drop. This paper examines the consequences of nonuniform gas distribution on conversion and selectivity for reactions described by simple kinetic rate expressions in both isothermal and adiabatic systems.

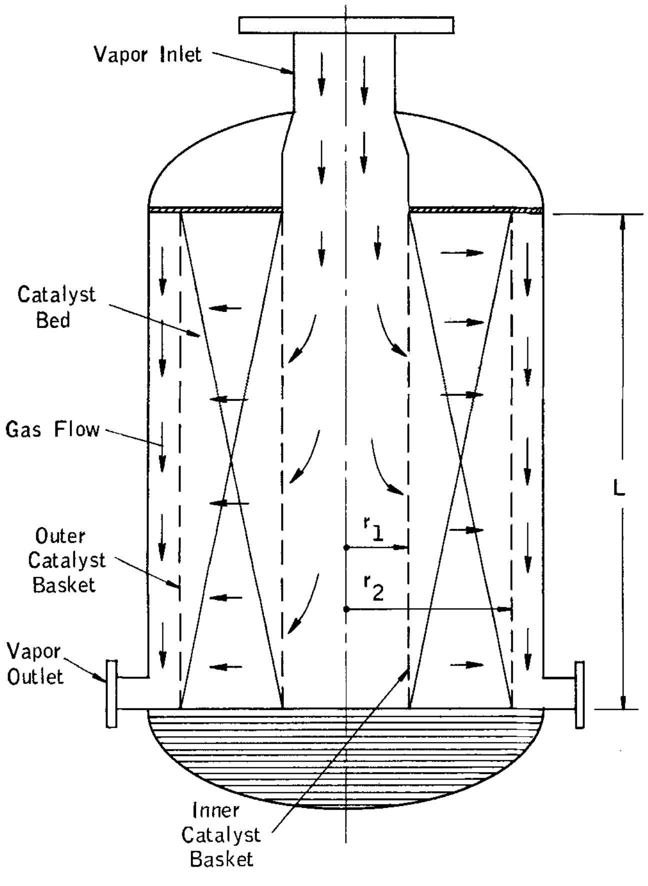


Fig. 1. Typical radial flow reactor configuration.

The general radial reactor configuration is shown in Figure 1. The gas flows in a radial direction across the catalyst which is retained in an annular region by perforated baskets. There are four possible flow orientations that can be used: from the central pipe outward or from the periphery inward, and concurrent or countercurrent.

Consider an axial element of the reactor as shown in Figure 2. For gas flow from the central pipe outward, the superficial velocity at the inner retaining baskets can be related to the axial velocity in the central pipe by the continuity expression

$$V_r(y) = \frac{-r_1}{2}\frac{W_o}{L}\frac{du}{dy} \tag{1}$$

From this equation, it can be seen that the flow of gas to all elements of the catalyst bed will be equal if du/dy has an absolute magnitude of unity. Furthermore, the maldistribution of the gas phase along the axial length of the bed is directly related to the deviation of the magnitude of du/dy from unity.

Dil'man et al. (1971) and Genkin et al. (1973) developed a model to predict the axial velocity profiles in radial reactors. The model was extended by Kaye (1978). Typical dimensionless velocity distributions are

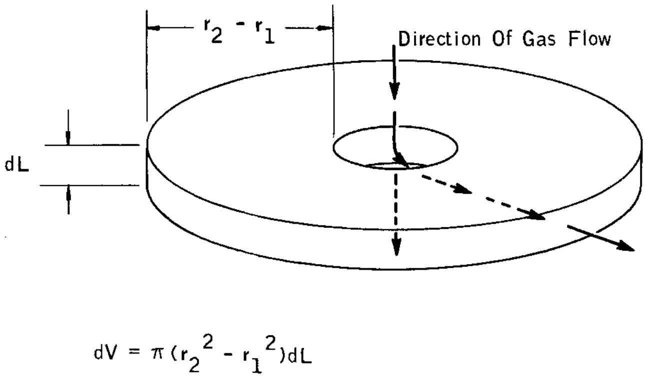


Fig. 2. Differential radial reactor catalyst element.

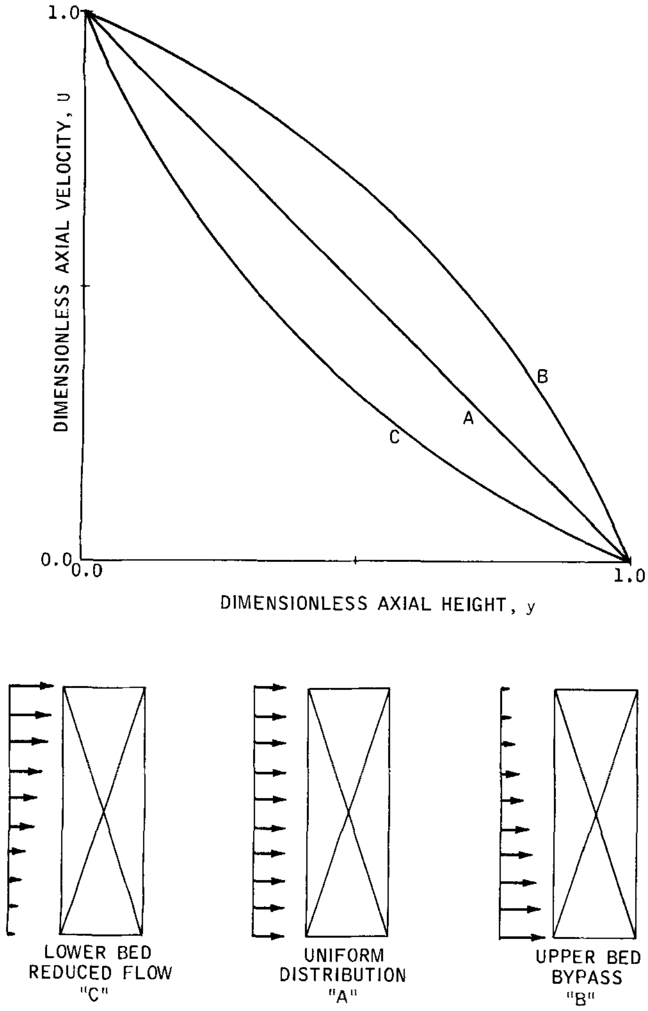


Fig. 3. Typical axial velocity distribution in flow channel upstream of bed.

presented in Figure 3 as a function of the dimensionless axial position. Curve A represents a uniform distribution with $du/dy = -1$ (the negative sign represents a decreasing velocity from the top to the bottom of the bed). Curves B and C depict maldistributed flows. Also shown schematically in Figure 3 is the corresponding fraction of the gas flow passing through the bed as a function of the axial bed height. For the case represented by curve B, the bulk of the gas flow bypasses the top of the bed, while in curve C the bottom part of the bed receives a decreased flow.

The effect of maldistribution on the conversion and selectivity of a reaction can be determined from a simple model in which the gas moves radially in plug flow fashion through an infinite array of parallel differential elements of the catalyst bed without axial flow by either convection or dispersion and without radial dispersion in the bed. The residence time in each of the differential elements is determined by the distribution of gas to the bed which is a function of the axial distance from the reactor inlet. The constraint imposed upon the system at a specific conversion level is that the residence time of the total gas flow is fixed. Thus, by varying the distribution of residence times to the individual elements by the degree of maldistribution, the effect of maldistribution at fixed total residence time can be studied. By varying the total residence time, the maldistribution effect can be studied at all levels of conversion.

The validity of the assumption of a negligible effect of axial flow within the bed will depend on the length to thickness ratio of the bed. If this ratio is high, radial gradients will predominate over axial, and the bed will have little effect on the maldistribution. Since axial flow by either dispersion or convection will tend to reduce gas maldistribution, the simple model used here will give conversion and selectivity effects which are the maximum possible for the case where radial dispersion is neglected. Radial dispersion in radial flow reactors with no feed maldistribution was studied by Lamba and Dudukovic (1975).

For the element shown in Figure 2, the conversion can be written (for zero initial conversion) as

$$\frac{V_i}{F_i} = \int_0^{x_{fi}} \frac{dx_i}{r_i} \tag{2}$$

If we assume no change in the number of moles upon reaction, the conversion in the total reactor is

$$F_T x_{fm} = \sum_i F_i x_{fi} \tag{3}$$

The subscript m indicates that the total conversion may be the result of a maldistributed flow. In the limit of a differentially small element, the summation in (3) can be replaced by an integral

$$x_{fm} = \frac{1}{F_T} \int_0^{F_T} x_f(y)\, dF \tag{4}$$

For flow from the central pipe outward, the differential flow of gas is

$$dF = 2\pi r_1 C_o L V_r(y)\, dy \tag{5}$$

Combining (1), (4), and (5), we get

$$x_{fm} = \int_0^1 \left(\frac{-du}{dy}\right) x_f(y)\, dy \tag{6}$$

The model is thus equivalent to a segregated flow model, where the fraction of gas entering the bed between y and $(y + dy)$ is given by $(-du/dy)dy$. By using the relationship given below between the average residence time $\bar{\tau}$ and the residence time in an element τ, the residence time distribution $p(\tau)$ for the flow may be obtained, since $(-du/dy)dy = p(\tau)d\tau$.

For a given reaction rate expression, $x_f(y)$ will be a function of the residence time in the differential element at position y. By definition

$$\tau(y) = \frac{C_o dV}{dF} \tag{7}$$

If we use (5), this relationship becomes

$$\tau(y) = \frac{(r_2^2 - r_1^2)}{2 r_1 V_r(y)} \tag{8}$$

Substituting the expression for $V_r(y)$ from (1), we get

$$\tau(y) = \frac{(r_2^2 - r_1^2)L}{r_1^2 W_o \left(-\frac{du}{dy}\right)} \tag{9}$$

However, for the entire reactor

$$\bar{\tau} = \frac{(r_2^2 - r_1^2)L}{r_1^2 W_o} \tag{10}$$

Therefore

$$\tau(y) = \frac{\bar{\tau}}{\left(\frac{-du}{dy}\right)} \tag{11}$$

Equations (2), (6), and (11) are used to calculate the

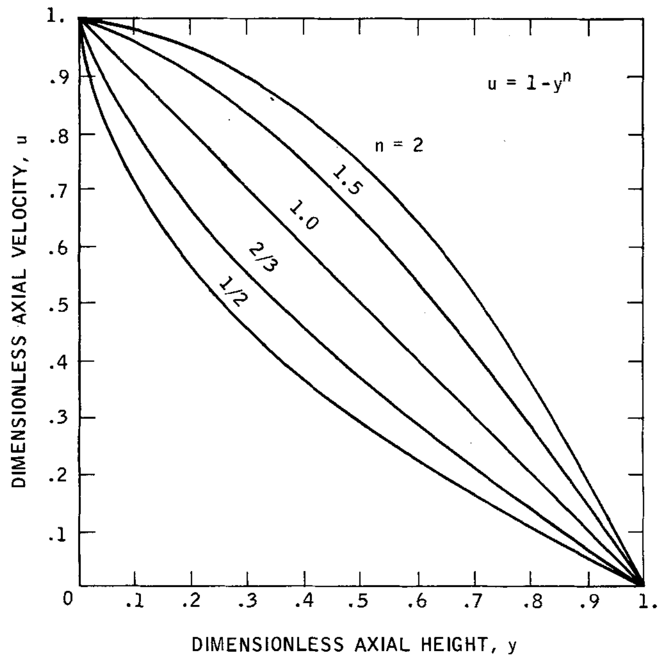


Fig. 4. Maldistribution in a radial flow reactor as a function of *n*.

overall conversion for a maldistributed flow with a specific reaction. For isothermal operation and simple kinetic expressions, analytical results can be developed. For adiabatic conditions, a numerical evaluation scheme is required.

Maldistributions, such as those depicted in Figure 3, will be approximated for purposes of this paper by an equation of the form

$$u = 1 - y^n \tag{12}$$

This approximation represents actual maldistributions quite well. Values of $n > 1$ can be used to simulate flow represented by curve B (Figure 3), while $0 < n < 1$ simulates the flow depicted by curve C. A uniform distribution results when n equals unity. The degree of maldistribution increases the more n deviates from a value of 1. Maldistributions described by Equation (12) are shown in Figure 4 for various values of n.

ISOTHERMAL OPERATION

As an illustration, consider a second-order, irreversible reaction. From (2) and (11) the final conversion, assuming zero initial conversion and no change in moles, will be

$$x_f(y) = \frac{\dfrac{k_{\bar{T}} C_o}{\left(\dfrac{-du}{dy}\right)}}{\dfrac{k_{\bar{T}} C_o}{\left(\dfrac{-du}{dy}\right)} + 1} \tag{13}$$

Substituting (13) into (6) and rearranging, we get

$$x_{f_m} = k_{\bar{T}} C_o \int_0^1 \frac{dy}{1 + \dfrac{k_{\bar{T}} C_o}{\left(\dfrac{-du}{dy}\right)}} \tag{14}$$

Choosing $n = 2$ in (12), we get

$$x_{f_m} = 2 k_{\bar{T}} C_o \int_0^1 \frac{dy}{2y + k_{\bar{T}} C_o} \tag{15}$$

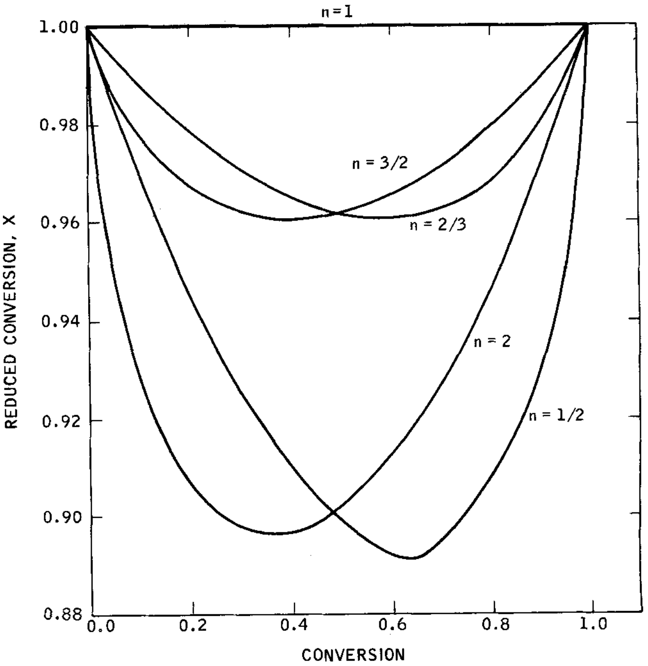


Fig. 5. Reduced conversion for second-order reaction systems with maldistribution.

which, on integration, gives

$$x_{f_m} = k_{\bar{T}} C_o + \frac{(k_{\bar{T}} C_o)^2}{2} \ln\left(\frac{k_{\bar{T}} C_o}{k_{\bar{T}} C_o + 2}\right) \tag{16}$$

Thus, with $n = 2$, the model is equivalent to the results of the axial laminar flow reactor model given in Aris (1969).

Figure 5 is a plot of X, the ratio of the conversion predicted by (16) divided by the conversion associated with uniform distribution as a function of the latter. Also shown in this figure are curves for other degrees of maldistribution. The debit to conversion due to maldis-

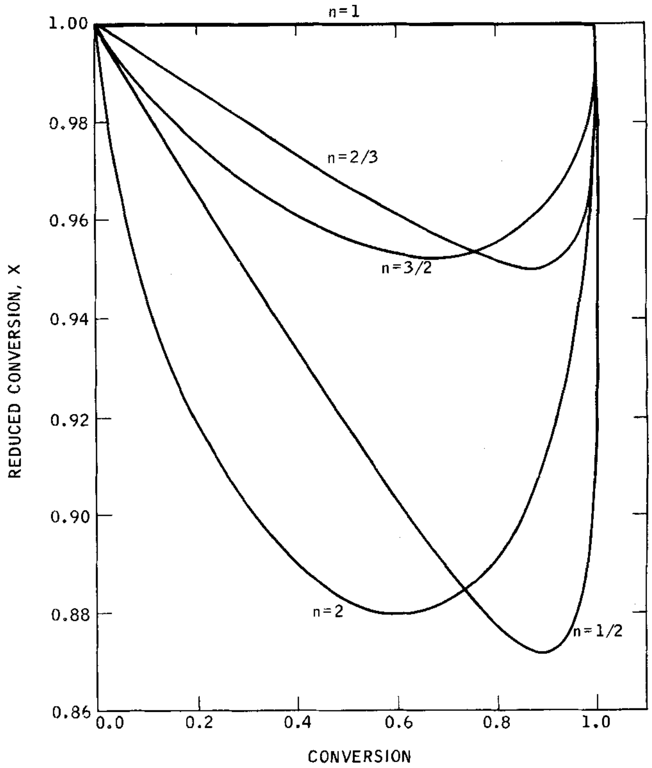


Fig. 6. Reduced conversion for first-order reaction systems with maldistribution.

TABLE 1. GENERALIZED EQUATIONS FOR CONVERSION AS A FUNCTION OF MALDISTRIBUTION FOR FIRST- AND SECOND-ORDER ISOTHERMAL REACTIONS WITH ZERO INITIAL CONVERSION AND NO CHANGE IN MOLES

Maldistribution described by $u = 1 - y^n$

First-order reaction

$n > 1$

$$x_{fm} = 1 + \frac{n}{1-n}\left(\frac{k\bar{\tau}}{n}\right)^{\frac{n}{n-1}} \Gamma\left(\frac{n}{1-n}, \frac{k\bar{\tau}}{n}\right)$$

where Γ is an incomplete gamma function defined by

$$\Gamma(a, x) = \int_x^\infty e^{-t} t^{a-1}\, dt$$

and evaluated with the infinite series given by Erdelyi (1953):

$$\Gamma(a, x) = \Gamma(a) - \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \frac{x^{a+n}}{(a+n)}$$

For the special values of n given by $n = \frac{j+1}{j}$, $j = 1, 2, \ldots$

$$x_{fm} = 1 + \frac{n}{1-n} E_{\left(\frac{1-2n}{1-n}\right)}\left(\frac{k\bar{\tau}}{n}\right)$$

where $E_{\left(\frac{1-2n}{1-n}\right)}$ is the exponential integral of order $\left(\frac{1-2n}{1-n}\right)$

$0 < n < 1$

$$x_{fm} = 1 - \frac{n}{1-n}\left(\frac{k\bar{\tau}}{n}\right)^{\frac{n}{n-1}} \gamma\left(\frac{n}{1-n}, \frac{k\bar{\tau}}{n}\right)$$

where γ is an incomplete gamma function defined by

$$\gamma(a, x) = \int_0^x e^{-t} t^{a-1}\, dt, a > 0$$

with

$$\gamma(a, x) = \sum_{n=0}^{\infty} \frac{(-1)^n x^{a+n}}{n!\,(a+n)}$$

For the special values of n given by $n = \frac{j}{j+1}$, $j = 1, 2, \ldots$

$$x_{fm} = 1 - \left(\frac{k\bar{\tau}}{n}\right)^{\frac{n}{n-1}} \left(\frac{n}{1-n}\right)! \left[1 - \exp\left(\frac{-k\bar{\tau}}{n}\right) \sum_{m=0}^{\left(\frac{2n-1}{1-n}\right)} \frac{\left(\frac{k\bar{\tau}}{n}\right)^m}{m!}\right]$$

Second-order reaction

$n > 1$

$$x_{fm} = \left(\frac{k\bar{\tau}C_o}{n + k\bar{\tau}C_o}\right) F\left(1, 1;\ \frac{2n-1}{n-1};\ \frac{n}{n + k\bar{\tau}C_o}\right)$$

where $F(a, b; c; z)$ is the hypergeometric function, Erdelyi (1953), with infinite series given by

$$F(a, b; c; z) = \sum_{n=0}^{\infty} \frac{(a)_n (b)_n}{(c)_n\, n!} z^n, \quad c \neq 0, -1, -2, \ldots \quad (a)_o = (b)_o = (c)_o = 1$$

and

$$(x)_n = \frac{\Gamma(x+n)}{\Gamma(x)} = x(x+1)\ldots(x+n-1), n = 1, 2, \ldots$$

As a special case, $n = \frac{j+1}{j}$, $j = 1, 2, \ldots$

then $\frac{2n-1}{n-1} = j + 2$, an integer

For $0 < n < 1$

The general expression is

$$x_{fm} = \left(\frac{n k\bar{\tau}C_o}{n + k\bar{\tau}C_o}\right) F\left(1, 1;\ \frac{2-n}{1-n};\ \frac{k\bar{\tau}C_o}{n + k\bar{\tau}C_o}\right)$$

For $n = \frac{j}{j+1}$, $j = 1, 2, \ldots$

then $\frac{2-n}{1-n} = j + 2$

For the special cases $n > 1$ and $0 < n < 1$, $F(1, 1; j + 2; z)$ may be expressed as a function of z and $\ln(1 - z)$ using the following relations:

$$F(1, 1; 1; z) = \frac{1}{1-z}$$

$$F(1, 1; 2; z) = -\frac{1}{z}\ln(1-z)$$

and

$$F(1, 1; c+1; z) = \frac{1}{(c-1)^2 z}[c(c-1)(1-z)F(1, 1; c-1; z) - c(c-1-(2c-3)z)F(1, 1; c; z)]$$

tribution is a function of the conversion level and increases as the maldistribution becomes worse, that is, as n increases from 1 for $n > 1$ and as n decreases from 1 for $0 < n < 1$. For the cases considered, this debit could be as much as 11%.

Figure 6 shows the maldistribution effect for a simple first-order reaction. Comparison of Figures 5 and 6 shows a slightly greater effect for first-order than for second-order reaction. As in Figure 5, the greater the maldistribution, the larger is the debit to conversion.

Generalized equations were developed which permit calculation of the conversion as a function of the maldistribution level n for first- and second-order isothermal reactions with no initial conversion and no change in moles and for flow from the central pipe outward. The equations are presented in Table 1.

SELECTIVITY EFFECTS

In addition to its use to determine conversion effects, the simple plug flow model can be used to study the effects of flow maldistribution on product selectivity. Consider the first-order, irreversible, isothermal reaction sequence described by

$$A \xrightarrow{k_1} R \xrightarrow{k_2} S$$

Table 2. Generalized Equations for C_{Rm}/C_{A_o} for Series Reaction as a Function of Maldistribution

Maldistribution described by $u = 1 - y^n$

$n > 1, k_1 \neq k_2$

$$\frac{C_{Rm}}{C_{A_o}} = \left(\frac{k_1}{k_2 - k_1}\right)\left(\frac{n}{1-n}\right)\left[\left(\frac{k_2\bar{\tau}}{n}\right)^{\frac{n}{n-1}} \Gamma\left(\frac{n}{1-n}, \frac{k_2\bar{\tau}}{n}\right) - \left(\frac{k_1\bar{\tau}}{n}\right)^{\frac{n}{n-1}} \Gamma\left(\frac{n}{1-n}, \frac{k_1\bar{\tau}}{n}\right)\right] \tag{A}$$

for $n = \dfrac{j+1}{j}, j = 1, 2, \ldots$

$$\frac{C_{Rm}}{C_{A_o}} = \left(\frac{k_1}{k_2 - k_1}\right)\left(\frac{n}{1-n}\right)\left[E_{\left(\frac{1-2n}{1-n}\right)}\left(\frac{k_2\bar{\tau}}{n}\right) - E_{\left(\frac{1-2n}{1-n}\right)}\left(\frac{k_1\bar{\tau}}{n}\right)\right]$$

$n > 1, k_1 = k_2 = k$

$$\frac{C_{Rm}}{C_{A_o}} = \left(\frac{n}{n-1}\right)\left(\frac{k\bar{\tau}}{n}\right)^{\frac{n}{n-1}} \Gamma\left(\frac{1}{1-n}, \frac{k\bar{\tau}}{n}\right)$$

for $n = \dfrac{j+1}{j}, j = 1, 2, \ldots$

$$\frac{C_{Rm}}{C_{A_o}} = \left(\frac{k\bar{\tau}}{n-1}\right) E_{\left(\frac{n}{n-1}\right)}\left(\frac{k\bar{\tau}}{n}\right)$$

$0 < n < 1, k_1 \neq k_2$

Same as (A) with $\Gamma\left(\dfrac{n}{1-n}, \dfrac{k\bar{\tau}}{n}\right)$ replaced by $\gamma\left(\dfrac{n}{1-n}, \dfrac{k\bar{\tau}}{n}\right)$

for $n = \dfrac{j}{j+1}, j = 1, 2, \ldots$

$$\frac{C_{Rm}}{C_{A_o}} = \left(\frac{k_1}{k_2 - k_1}\right)\left(\frac{n}{1-n}\right)!\left[\left(\frac{k_2\bar{\tau}}{n}\right)^{\frac{n}{n-1}}\left[1 - \exp\left(\frac{-k_2\bar{\tau}}{n}\right)\sum_{m=0}^{\left(\frac{2n-1}{1-n}\right)} \frac{\left(\frac{k_2\bar{\tau}}{n}\right)^m}{m!}\right] - \left(\frac{k_1\bar{\tau}}{n}\right)^{\frac{n}{n-1}}\left[1 - \exp\left(\frac{-k_1\bar{\tau}}{n}\right)\sum_{m=0}^{\left(\frac{2n-1}{1-n}\right)} \frac{\left(\frac{k_1\bar{\tau}}{n}\right)^m}{m!}\right]\right]$$

$0 < n < 1, k_1 = k_2 = k$

$$\frac{C_{Rm}}{C_{A_o}} = \left(\frac{n}{1-n}\right)\left(\frac{k\bar{\tau}}{n}\right)^{\frac{n}{n-1}} \gamma\left(\frac{1}{1-n}, \frac{k\bar{\tau}}{n}\right)$$

for $n = \dfrac{j}{j+1}, j = 1, 2, \ldots$

$$\frac{C_{Rm}}{C_{A_o}} = \left(\frac{n}{1-n}\right)\left(\frac{k\bar{\tau}}{n}\right)^{\frac{n}{n-1}}\left(\frac{n}{1-n}\right)!\left[1 - \exp\left(\frac{-k\bar{\tau}}{n}\right)\sum_{m=0}^{\frac{n}{1-n}} \frac{\left(\frac{k\bar{\tau}}{n}\right)^m}{m!}\right]$$

As shown by Levenspiel (1972), the ratio of the concentration of the intermediate product R to the initial concentration of A, assuming no R or S present initially, is given by

$$\frac{C_R}{C_{A_o}} = \frac{k_1}{k_2 - k_1}\left[\exp(-k_1\tau) - \exp(-k_2\tau)\right], \quad k_1 \neq k_2 \tag{17}$$

and

$$\frac{C_R}{C_{A_o}} = k_1\tau\exp(-k_1\tau), \quad k_1 = k_2 \tag{18}$$

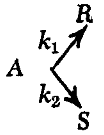
If we follow the same line of reasoning as used to obtain (6), the intermediate concentration for the case where the gas flow is maldistributed is

$$C_{R_m} = \int_0^1 \left(\frac{-du}{dy}\right) C_R(y)dy \tag{19}$$

where $C_R(y)$ is obtained by substituting $\bar{\tau}/(-du/dy)$ for τ in (17) and (18). Analytical expressions for C_{R_m}/C_{A_o} for any $n > 0$ are presented in Table 2.

Figure 7 presents plots of C_R/C_{A_o} as a function of $k_1\bar{\tau}$ for a uniform distribution and various maldistributions for k_2/k_1 equal to 0.1, 1.0, and 10.0, respectively. The figure shows that in certain ranges of $k_1\bar{\tau}$ it is possible to have a higher production of R with maldistributed flows. Maximum production is obtained, however, with a uniformly distributed flow in a reactor with the most appropriate residence time.

The case of a first-order, irreversible, parallel reaction may be treated most simply by noting that for



the concentration of C_{R_m} is given by

$$C_{R_m} = \frac{k_1}{k_1 + k_2} C_{A_o} x_{f_m} \tag{20}$$

where x_{f_m} is obtained from the equations given in Table 1 for a first-order reaction with $k_1 + k_2$ substituted for k.

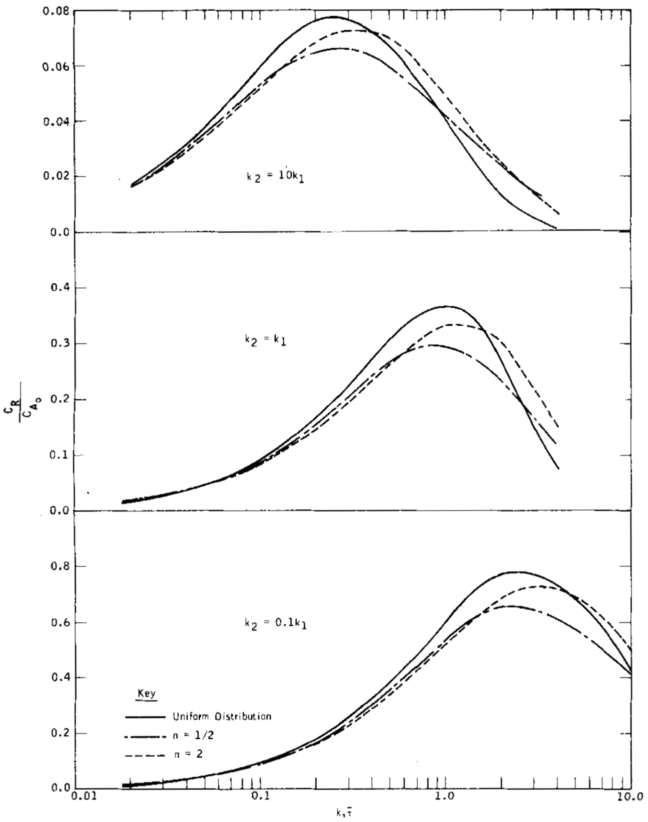


Fig. 7. The effect of maldistribution on selectivity for $A \xrightarrow[k_1]{} R \xrightarrow[k_2]{} S$.

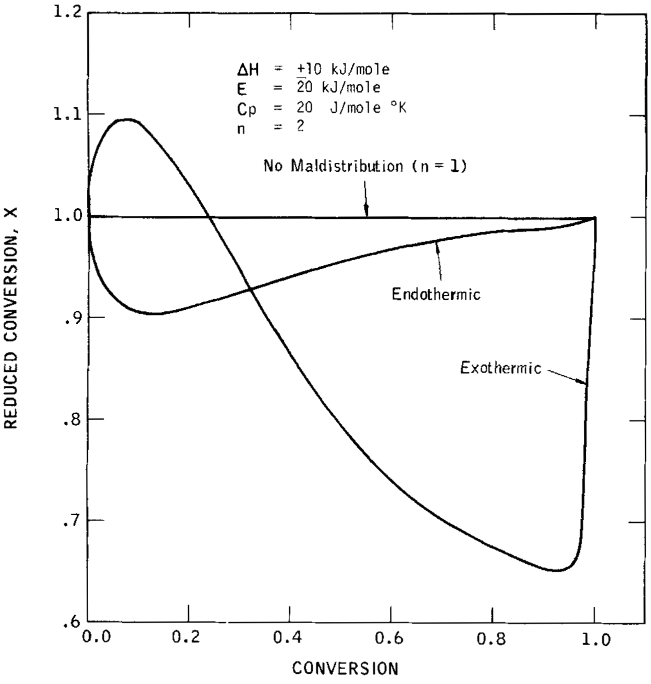


Fig. 8. Effect of maldistribution in adiabatic reactors.

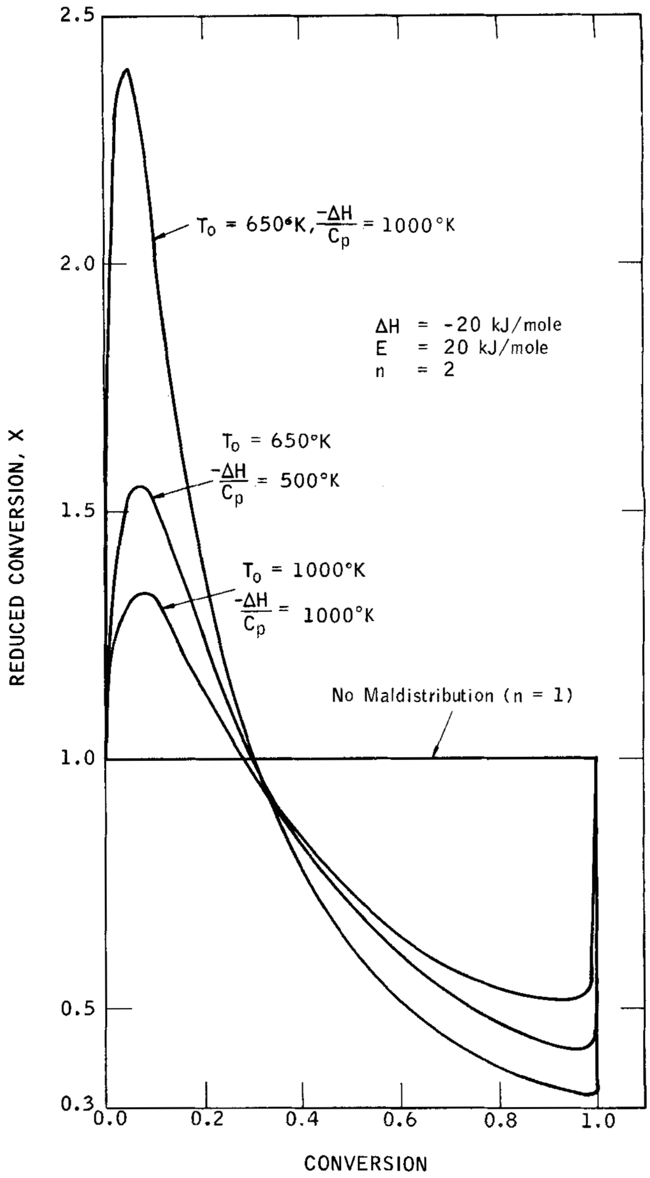


Fig. 9. Effect of T_o and $\Delta H/C_p$ on conversion with gas maldistribution for an exothermic first-order reaction.

ADIABATIC OPERATION

The simple model for determining the maldistribution effect on conversion in a radial reactor can be extended to include adiabatic operations. The effects, however, must be determined numerically.

Again, consider the differential element of catalyst bed which receives a given flow of gas from the central pipe. Assume that the gas temperature is T_o and the initial conversion is zero. Then, for a first-order reaction with constant density

$$r = k_oC_o(1 - x)\exp\left(\frac{-E}{RT}\right) \tag{21}$$

Assuming no loss of heat from the element, T can be related to conversion by

$$T = T_o + \frac{(-\Delta H)}{C_p}x \tag{22}$$

Substituting (21) and (22) into (2), we get

$$\frac{k_oC_oV_i}{F_i} = \int_0^{x_{fi}} \frac{dx_i}{(1 - x_i)\exp\left[\frac{-E}{R\left(T_o + \frac{(-\Delta H)}{C_p}x_i\right)}\right]} \tag{23}$$

As shown by Douglas and Eagleton (1962), this equation may be integrated to give for a differential element

$$k_{oT}(y) = Ei\left[\frac{E}{R\left(T_o + \frac{(-\Delta H)x_f(y)}{C_p}\right)}\right]$$

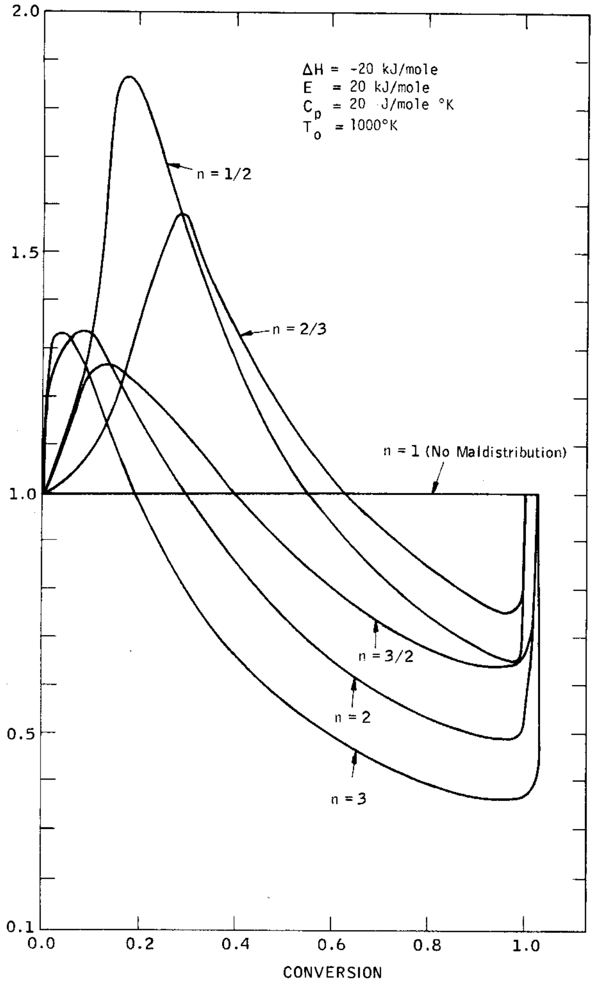


Fig. 10. The effect of degree of maldistribution on conversion for a first-order exothermic reaction.

$$\begin{aligned}
&-Ei\left[\frac{E}{RT_o}\right]+\exp\left[\frac{E}{R\left(T_o+\dfrac{(-\Delta H)}{C_p}\right)}\right]\\
&\quad\Bigg[Ei\Bigg(\frac{E}{RT_o}-\frac{E}{R\left(T_o+\dfrac{(-\Delta H)}{C_p}\right)}\Bigg]\\
&\quad-Ei\Bigg(\frac{E}{R\left(T_o+\dfrac{(-\Delta H)x_f(y)}{C_p}\right)}\\
&\qquad-\frac{E}{R\left(T_o+\dfrac{(-\Delta H)}{C_p}\right)}\Bigg]\Bigg]
\end{aligned}\tag{24}$$

The integration of (6) to obtain x_{f_m} was done numerically utilizing a graph of $k_o\tau(y)$ as a function of $x_f(y)$ generated by using (24). The integrand in (6) was calculated at discrete values of y for a given k_o using (11) and this graph to obtain $x_f(y)$.

Cases were developed for first-order kinetics to show the effect of $(-\Delta H)/C_p$, T_o, and E on conversion. The results are shown for endothermic and exothermic systems ($\Delta H = \pm 10$ kJ/mole, $C_p = 20$ kJ/mole °K, $T_o = 1\,000$°K, and $E = 20$ kJ/mole) in Figure 8, where X is plotted vs. the conversion obtained with uniformly distributed feed.

For the exothermic case, the conversion with a maldistributed flow can be appreciably greater than for uniform gas distribution at low conversion levels. This enhancement is attributable to the higher temperature utilization of some sections of the catalyst bed. For higher conversion level reactors, the maldistribution debit offsets any enhancement.

In general, the maldistribution effects on conversion become more pronounced with increasing values of $\Delta H/C_p$ and maldistribution and with decreasing values of T_o. Some typical curves demonstrating these sensitivities are shown in Figures 9 and 10 for an exothermic system. It should be remembered that the conversion effects predicted are maximum values. Heat losses from the bed, dispersion of heat and mass, axial flow of gas, and catalyst deactivation at high temperature will all tend to make the effects less pronounced. A more accurate analysis of flow maldistribution would require the solution of the heat and mass balance equations which take dispersion and gas convection due to axial pressure gradients into account.

NOTATION

C = concentration, mole/m^3
C_p = molar specific heat, J/mole °K
E = activation energy, kJ/mole
Ei = exponential integral
F = molar feed rate, mole/s
ΔH = heat of reaction, kJ/mole
k = rate constant, (m^3/mole)$^{\text{reaction order}-1}$s^{-1}
k_o = preexponential factor, (m^3/mole)$^{\text{reaction order}-1}$s^{-1}
L = axial catalyst bed length, m
n = power of y in velocity distribution equation
$p(\tau)$ = residence time distribution of gas, s^{-1}
r = reaction rate based on bed volume, mole/m^{3}s
R = gas constant, J mole^{-1} °K^{-1}
r_1 = central pipe radius, m
r_2 = outer bed radius, m
T = temperature, °K
u = W/W_o, axial velocity in central pipe, dimensionless
V_r = superficial radial velocity at inner basket, m/s
V = volume of fixed bed, m^3
W = central pipe axial velocity, m/s
x = conversion
X = ratio of conversion obtained with maldistributed flow to conversion obtained with uniformly distributed flow
y = axial length, dimensionless
τ = residence time in an element, s
$\bar{\tau}$ = average residence time for whole reactor, s

Subscripts

A, R, S = species designations
f = final value
i = i^{th} element
m = maldistributed
o = initial value, referring either to entrance to inner pipe at inlet of reactor or to entrance radially to catalyst bed from inner pipe
T = total

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Safety and Reliability Synthesis of Systems with Control Loops

A method of a reliability synthesis for a system with control loops is proposed by introducing a concept which we call a critical transition set. The set is an extended set of an exact failure mode and is important in that each occurrence of the system failure has to correspond to a mode in the set. This means that the system can be improved in such a way as to eliminate all the dominant modes in the set.

First, the system diagram is obtained by connecting outputs of components to the inputs of succeeding components. Time delays are introduced in the feedback loops to represent the internal system state (memory). Then, the components are modeled by decision tables. The critical transition set can be obtained easily by simple tabular manipulations once the system failure is defined. Finally, the system reliability and availability improvements are made based on the set.

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SCOPE

This paper develops a new method for obtaining reliability and safety parameters for process systems containing control loops. It is based on the construction of decision tables for the individual components in a process flow sheet, followed by a series of tabular manipulations to eliminate the internal variables and yield the critical transition modes. These are analogous to cut sets and can be used to obtain reliability and safety parameters. Systems can be upgraded and improved by eliminating one-event critical modes and/or modes in which the combined probabilities of failure are undesirably high.

Feedback and feed forward control loops are handled by introducing time delays which represent internal memory. Given an adequate library of component decision tables, the synthesis of large systems can be readily automated, the safety analyst being relieved to the tedium of constructing system fault trees.

CONCLUSIONS AND SIGNIFICANCE

The construction of fault trees to obtain top-event parameters such as reliability, availability, and expected number of failures is a well-established practice in the nuclear and aerospace industries which is being widely adopted in the process industries. Their construction is time consuming; several man years are required to produce a tree for a nuclear power plant. Furthermore, the trees become extremely complicated, errors frequently occur, and the work is tedious and often nonproductive. Another problem is that systems containing control loops are not analyzable by presently available techniques because they lead to logic complexities, problems of state history, and, ultimately, to trees that are not coherent and for which top-event probabilities can not be rigorously calculated.

What is required is a computer based synthesis procedure by which the top-event probabilities for a complicated process flow sheet can be synthesized from "Mini-Fault Trees" which represent the components (including control loops). One such method, based on digraphs, has recently been proposed. This, however, is heuristic in nature and leads to fault trees which are difficult to interpret quantitatively or qualitatively and are not necessarily correct.

In this paper we propose a method for synthesizing system failure modes which is based on decision tables for the individual components. It produces, instead of fault trees, a table of critical transition modes which represent the unique system failure modes. These modes can be used, like cut sets, for improving system safety and for calculating top-event probabilities. The methodology lends itself readily to computer automation.

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