nate, 2 for radial cylindrical coordinate, and 3 for radial spherical coordinate

min, max = limits of particle size modulus for multiple solution region

0 = outer surface

1 = first collocation approximation, or first eigenvalue

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A Stochastic Analysis of a Nonisothermal Packed Bed Reactor

Monte Carlo techniques have been used to simulate the stochastic responses of the nonisothermal packed bed reactor. Random variables with specified ensemble means, ensemble standard deviations, and probability distributions (normal, uniform, or autocorrelated) were introduced as inputs and parameters into the model equations, and the equations were solved repeatedly to provide a sample of the outputs. Sample means and sample standard deviations both in the steady and unsteady state were evaluated and the probability distributions of the output temperature and concentration characterized. Confidence limits for a specified confidence coefficient have been determined from which overdesign factors could be computed.

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SCOPE

In formulating a mathematical model of a process, two different approaches can be discerned: one is deterministic and the other stochastic. In a stochastic model a knowledge of the state of the variables and parameters at some moment in time no longer uniquely determines the state of the parameters at succeeding times. Stochastic models are, in general, more difficult to work with than deterministic models, but in many cases they can provide more insight into the characteristics and behavior of a real process.

Unfortunately, but not unexpectedly, the formulation of the more representative stochastic models of reactors results in equations whose dependent variables are non-Markovian, nonstationary or both. Consequently, while it is usually not too difficult to write down the basic (differential) equations describing a packed bed reactor, how to obtain a complete, partial, or approximate analytical solution for a stochastic reactor model is a stumbling block. Most of the published work on reactor models has been limited to the somewhat unrealistic case in which the random coefficients and inputs are white noise because then analytical solutions can be found.

One way to handle more realistic random inputs and parameters is to obtain approximate solutions for the moments and distributions of the model response via Monte Carlo simulation. This type of analysis permits the comparison of the output of the stochastic reactor model with the output of the deterministic model in order to ascertain if there are any differences, and it provides information about the degree of uncertainty in the modeled process (the dispersion of the responses). The latter information can be used to compute overdesign or safety factors. By knowing the desired conversion of a chemical species in a tubular reactor and by specifying the confidence coefficient, it is possible to calculate how much additional volume is needed for the reactor in comparison to the reference volume calculated from the deterministic model.

This investigation was devoted to a stochastic analysis of a nonisothermal tubular packed bed reactor. The general objectives of this study were:

To carry out Monte Carlo simulations and obtain the sample statistics of the output variables.

2. To examine the relative frequency distributions of the output temperature and concentration and to characterize their ensemble probability distributions.

3. To determine if the sample means of the model responses equaled the deterministic means obtained by solving the corresponding deterministic model.

4. To estimate the ensemble standard deviations of the model responses by calculating their sample standard deviations.

5. To calculate the confidence limits for the output variables from the sample means and the sample standard deviations and develop appropriate methods of computing overdesign factors.

CONCLUSIONS AND SIGNIFICANCE

The frequency distributions for the reactor concentration generally could be characterized by a normal probability density with one or two exceptions. The frequency distributions for the temperature were skewed considerably to left when each of ΔE, k_0, and ΔH was random. Otherwise, the distributions of T could be characterized by a normal probability density. As long as the distribution of an output was normal, standard tables could be used to estimate the confidence limits for the output, and extensive simulations would not be required to develop a special frequency distribution.

The sample means of the output concentration and temperature in both the unsteady and pseudo steady states were not significantly different from the corresponding deterministic solutions, with some exceptions, and such differences as existed were small enough that they could be ignored for engineering purposes. It was noted that changing the type of random variables used for the coefficients and input had no effect on the type of distribution of the output concentration and temperature. This meant that knowledge about the type of the probability distributions of the random process inputs and parameters was not critical in the analysis.

Uncertainty in the activation energy and T_W rather than v_Z, $\tilde{D}_A$, T_i, or C_{Ai} had the most significant effect on the sample standard deviations of output variables, and hence on the determination of overdesign factors.

The results presented here demonstrate how to use a stochastic analysis as a supplement to the usual deterministic design and achieve a more quantitative specification of uncertainty.

In packed bed tubular reactors, the concentrations and temperatures are random variables. Also, the parameters in the process models are never known exactly, but must be estimated from experimental data and are consequently random. One way to take into account this inherent feature of uncertainty in the reactor is to employ stochastic process models rather than the conventional deterministic ones. Such models provide a convenient and economical basis for studying the effect of changes in variables and operating conditions on the output of a real process in so far as the model can represent the real process.

Stochastic models evolve through two main routes. Some stochastic models, such as those used to represent flow in a porous reservoir, for example, can be derived by directly employing probabilistic concepts to small physical subdivisions of the process. An alternate method of obtaining stochastic models is to take a deterministic model and transform it into a stochastic model by introducing random variables either as inputs or as coefficients, or both. It is this alternate approach that will be used here. Neither route of approach is more correct than the other because the ultimate models are approximations in any case. But in each approach the engineer must take care to make the introduction of randomness in the model reflect what is happening physically in the process in so far as possible.

This work is part of a continuing study of the use of stochastic models in the analysis and design of chemical reactors. Only a few attempts have been made to apply stochastic models to processes of interest to the chemical engineer (Acrivos, 1960; Aris and Amundson, 1958; Homan and Tierney, 1960; Katz, 1958; King, 1968). One finds as a general rule that the statistics of the response of any but the simplest reactor models must be obtained via simulation. Berryman and Himmelblau (1971) described how Monte Carlo simulation can be used to study the effect of stochastic inputs and parameters on the responses of nonlinear models and examined the stochastic responses of well stirred tank and plug flow reactors (1973). In as much as the well stirred tank and plug flow reactors represent extremes of mixing, it was felt that an analogous study of the dispersed flow reactor would help fill in the gap. To this end Kado (1972) examined the isothermal dispersion reactor. Here we discuss a more complicated reactor, the nonisothermal tubular or packed bed reactor.

One major objective of the investigation was to characterize the responses of the nonisothermal tubular reactor in terms of their probability distributions. A second objective was to demonstrate how to use the information generated from simulation to estimate the degree of overdesign (oversizing) required for the reactor length or volume to meet the desired output performance specifications at a given probability level.

REACTOR MODEL

The nonisothermal reactor shown in Figure 1 has been discussed by Coste et al. (1961) and Liu (1967) from a deterministic viewpoint. Reactant A is introduced into the reactor at $z = 0$ and the first order, irreversible reaction $A \rightarrow B$ takes place in the reactor. It is assumed that the density of the fluid is constant; therefore, v_z is a constant fluid velocity throughout the reactor. The model partial differential equations are as follows:

$$\frac{\partial C_A}{\partial t} + v_z \frac{\partial C_A}{\partial z} = \tilde{D}_A \frac{\partial^2 C_A}{\partial z^2} - k_0 C_A \exp\left(-\frac{\Delta E}{RT}\right) \tag{1}$$

Energy balance

$$\frac{\partial T}{\partial t} + v_z \frac{\partial T}{\partial z} = \frac{\tilde{k}}{\rho C_p} \frac{\partial^2 T}{\partial z^2} - \frac{2U}{r\rho C_p}(T - T_w) - \frac{\Delta H}{\rho C_p} k_0 C_A \exp\left(-\frac{\Delta E}{RT}\right) \tag{2}$$

It is assumed that the thermal diffusivity is equal to the mass diffusivity (Coste, 1961).

$$\tilde{D}_A = \frac{\tilde{k}}{\rho C_p} \tag{3}$$

The boundary conditions are

At the inlet $z = 0, t > 0$

$$v_z C_{Ai} = v_z C_A - \tilde{D}_A \frac{\partial C_A}{\partial z} \tag{4}$$

$$v_z T_i = v_z T - \tilde{k}_A \frac{\partial T}{\partial z} \tag{5}$$

At the exit $z = L, t > 0$

$$\frac{\partial C_A}{\partial z} = 0 \tag{6}$$

$$\frac{\partial T}{\partial z} = 0 \tag{7}$$

and the initial conditions are

$$C_A = C_{A0} = 0 \tag{8}$$

$$T = T_0 \qquad t = 0,\ 0 \leq z \leq L \tag{9}$$

Not all of the variables in the model were permitted to be random. Table 1 lists the random inputs and parameters together with the types of distributions used for them. The inputs C_{Ai} and T were random time sequences while the coefficients $\tilde{D}_A$, k_0, ΔE, ΔH, U, and the fluid velocity v_z were assumed to be constant in one run but different in different runs. Although the random variable $v_z(t)$ should in principle be a random function of time in the process and in the model, a very tedious numerical technique would be required to treat $v_z(t)$ properly if it were made a function of time so that the $v_z(t)$ was not assumed to be a random function of time. The implications that pertain to this decision are as follows. In the plug flow model of a reactor no backward flow exists. However, in the dispersion model both forward and backward flow conceptually and physically exist. The basic assumption in the model used in this study was that v_z represented a net forward velocity represented by

$$v_z = u_z - w_z$$

where u_z was the forward fluid velocity and w_z was the backward velocity. Suppose that $v_z(t)$ is a function of time; let the time averaged flow velocity of $v_z(t)$ be denoted as $\tilde{v}_z$

$$\tilde{v}_z = \left[\sum_{j=1}^{M} v_{zj}(t)\right] \Big/ M \tag{10}$$

where $v_{zj}(t)$ represents the random fluid velocity in the time sequence and M is the number of changes of the fluid velocity per residence time. Now $v_{zj}(t)$ can be assumed to be composed of an expected value independent of time and a random component $Z_{v_{zj}}(t)$ that depends on time

$$v_{zj}(t) = E[v_z(t)] + Z_{v_{zj}}(t) \tag{11}$$

Substitution of Equation (11) into Equation (10) gives

$$\tilde{v}_z = E[v_z(t)] + \left[\sum_{j=1}^{M} Z_{v_{zj}}(t)\right] \Big/ M \tag{12}$$

When M is large, $\left[\sum_{j=1}^{M} Z_{v_{zj}}(t)\right] / M$ approaches zero.

Therefore, if the fluid velocity fluctuates very rapidly relative to the residence time, $v_z(t)$ can be treated as a constant for any Monte Carlo run. On the other hand, when the frequency of change of v_z is much larger than the residence time, $v_z(t)$ can also be treated as a constant. Therefore, in these two extreme cases v_z is not a function of time.

In the intermediate case, it is necessary to keep track of the time record of $v_{zj}(t)$, and the bookkeeping becomes quite cumbersome. Furthermore, the numerical solution of the finite difference approximation to the model becomes extremely complicated. Therefore, the results described here represent limiting cases but will not differ substantially from the case in which v_z is a function of time.

TABLE 1. CLASSIFICATION OF THE RANDOM VARIABLES

	Time dependent	Normal	Uniform	Auto-correlated
$\tilde{D}_A$	no	yes	no	no
v_z	no	yes	no	no
k_o	no	yes	no	no
ΔE	no	yes	yes	no
ΔH	no	yes	no	no
U	no	yes	no	no
C_{Ai}	yes	yes	yes	yes
T_i	yes	yes	no	yes
T_w	yes	yes	yes	yes

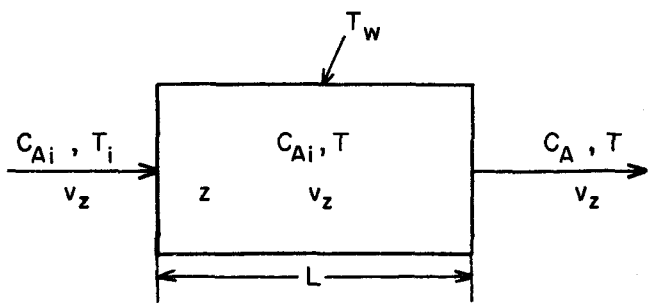

Fig. 1. Nonisothermal tubular or packed bed reactor

Table 2. Values of the Base Case Inputs and Parameters

Parameter	Deterministic value
$<P> = <v_z> L/<\tilde{D}_A>$	4 or 10
$<k_o> L/<v_z>$	$\exp(24.90768) = 6.5655 \times 10^{10}$
$(<\Delta E>/R)/<T_i>$	$10{,}757/340 = 31.638$
$(<\Delta H>/\rho C_p)(<C_{Ai}>/<T_i>)$	$7300(0.02/340) = 0.42941$
$(2<U>/\rho C_p)(L/<v_z>)$	0.0225
$<T_w>$	340°K
$<T_i>$	340°K
$<T_o>$	340°K

It was assumed that the wall temperature T_w was random in time, changing during one run, but was not a function of distance. The initial conditions C_{A0} and T_0 were fixed at 0 and 300(°K), respectively. Furthermore, it was assumed that the molar heat capacity C_p and mass density ρ were deterministic. To provide some realistic numbers to discuss, the ensemble (deterministic) physical quantities used in the examples cited here were taken from Coste et al., except that the $< P >$ was 4 or 10 compared with a value of 60 used by them; Table 2 lists the values of the base case parameters in dimensionless form (except for temperature).

Ensemble coefficients of variation (that is, the ensemble standard deviation divided by the ensemble average) for each of the coefficients and inputs were assumed to be large enough to be realistic and were as follows:

Random variables	Ensemble Coefficients of variation
$\tilde{D}_A$, k_0, ΔH, C_{Ai}, v_z	0.10
T_i	0.01
ΔE, T_w	0.005, 0.01, 0.02

The frequency of change of C_{Ai}, T_i, and T_w for the results to be described here was 10 changes per residence time unless otherwise stated. Higher frequencies of change, say 100, tend to introduce some damping of the random error because of the character of the mixing that takes place in the reactor, whereas low frequencies of change, say 1 per residence time, do not really represent a random variable. Figure 2 indicates how the frequency of change (per residence time) affected the output concentration. As the frequency of change of T_w became larger, $\hat{\gamma}_{C_A/C_{Ai}}$ became smaller. (The frequency of change of T_w of 0 in Figure 2 means that T_w did not change during one run, but this assumption would not represent physical reality.)

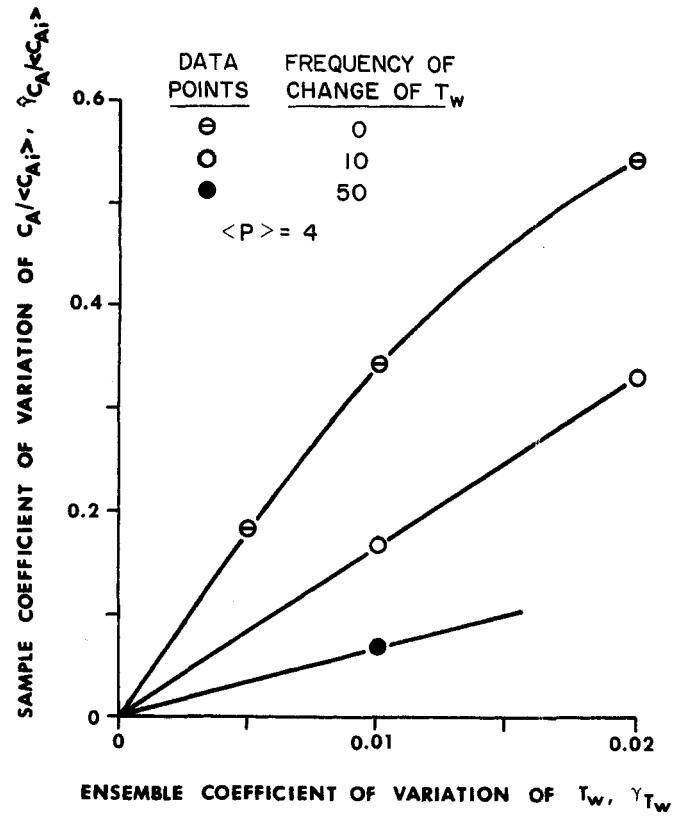

Fig. 2. $\hat{\gamma}_{C_A/<C_{Ai}>}$ vs. γ_{T_w} for the pseudo steady state ($t^* = 4$).

PROCEDURE

The specific procedure followed in this study can be outlined by the following three steps:

1. Generation of the appropriate random coefficients and random boundary conditions (or random inputs) of the given model as described in Berryman and Himmelblau (1971) where the computer programs are listed.
2. Repeated solution of the partial differential equations incorporating sequences of these random parameters. Appropriate finite difference approximations were used to obtain solutions for the dependent variables T and $(C_A/< C_{Ai} >)$ as a function of time and distance down the reactor.
3. Subsequently, the sample mean and sample standard deviation of the output (dependent) variables of the model were calculated at each sample point. In addition, the frequency distribution of the output variables at the outlet of reactor in the transient and pseudo steady states was examined and the probability distributions identified by appropriate statistical tests. In particular, the Kolmogarov-Simirnov and Chi-Squared tests for Goodness of Fit were used. It was concluded from an analysis of the errors of the first and second kind that a sample of 200 values would be adequate.

Steps (1), (2), and (3) consisted of one set of simulations, and they were repeated for various combinations of the ensemble dimensionless parameters and random variables.

RESULTS

The main points of interest that will be discussed here are:

1. What types of distributions were observed for the output temperature and concentration?
2. Did the sample means of the temperatures and concentrations differ from the corresponding deterministic means?
3. How sensitive were the distributions of temperature and concentration, and their expected values and dispersion, to changes in the assumptions about the probability distributions of the random inputs and parameters?
4. How could the information generated be used in reactor design?

Certain Unsteady State Results

The computation time for 200 runs each to reach $t^* = 4.0$, the pseudo steady state, was about 20 minutes.

(Because stochastic processes never reach the true steady state in the deterministic sense, we have termed times greater than $t^* = 4$ as the pseudo steady state.)

Figure 3 shows the sample means of $C_A/< C_{Ai} >$ and T obtained in the unsteady state when C_{Ai} was the only normal random variable for $< P > = 4$. Exactly the same type of results were obtained when ΔE was the only random variable and when several variables were random simultaneously. Observe that the sample means of $C_A/< C_{Ai} >$ and T followed the deterministic solution closely as was demonstrated by statistical tests. In Figure 3, the confidence limits of $C_A/< C_{Ai} >$ at $t^* = 3.0$ have been calculated based on the assumption that the distribution of $C_A/< C_{Ai} >$ could be represented by a normal distribution.

Because of limited space here and the greater importance of pseudo steady state operation, the remainder of the discussion of the results will be devoted to the responses for $t^* \geqq 4.0$. None of the conclusions reached for the pseudo steady state would be contradicted by the unsteady state observations.

Distribution of the Model Responses $C_A/< C_{Ai} >$ and T

Information about the character of the distributions of the model responses is important if the dispersions of the responses are to be used for design. The frequency distributions of $C_A/< C_{Ai} >$ and T, when each of U, $\tilde{D}_A$, v_z, C_{Ai}, T_i, or T_w was the only random variable, were symmetric about the sample means of $C_A/< C_{Ai} >$; figures showing these distributions can be found in Kado (1972). The null hypothesis that the distributions of $C_A/< C_{Ai} >$ and T could be represented by a normal distribution was tested and accepted at a significance level of 0.05 for most of the cases.

The only skewed frequency distribution of $C_A/< C_{Ai} >$ occurred when $\gamma_{\Delta E}$ was 0.02 (see Figure 4) but several skewed distributions for T were observed when either k_0,

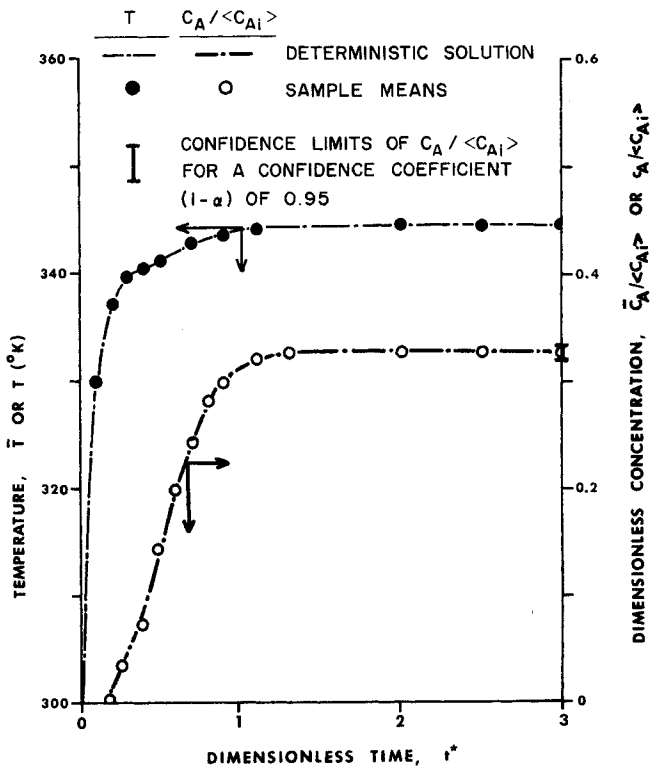

Fig. 3. Unsteady state response for $<P> = 4$ when C_{Ai} was the only random variable and normal, $\gamma_{CAi} = 0.10$

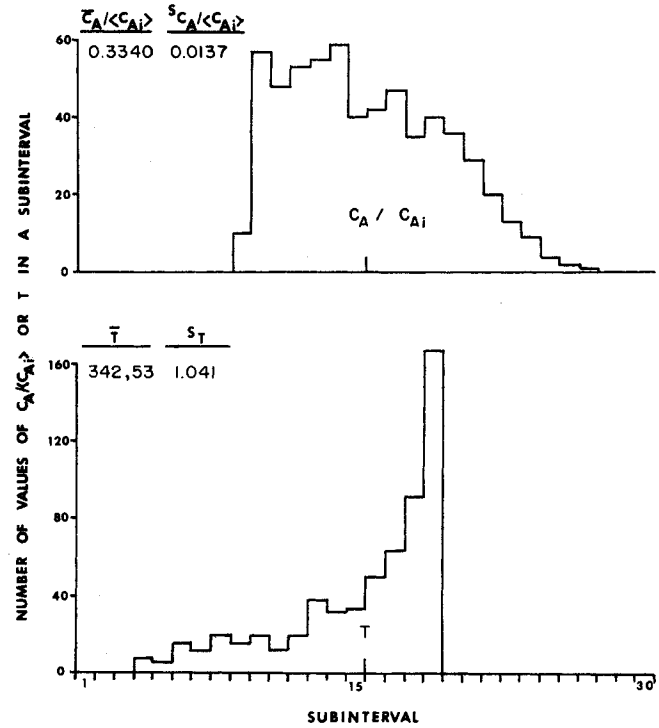

Fig. 4. Distribution of $C_A/<C_{Ai}>$ and T using normal generator for ΔE with $\gamma_{\Delta E} = 0.02$ in the pseudo steady state ($t^* = 4$) for a sample size = 600.

ΔE, or ΔH was the only random variable. One subinterval on the abscissa of Figure 4 is ¼ of the sample standard deviation of $C_A/< C_{Ai} >$ or T. The sample mean of $C_A/< C_{Ai} >$ or T was located at the point between subintervals 15 and 16. The reason for the skewness of $C_A/< C_{Ai} >$ is presumed to be as follows. The minimum and maximum concentrations of $C_A/< C_{Ai} >$ were 0.0009 and 0.938, respectively, while the sample mean was 0.334. Because $C_A/< C_{Ai} >$ could not be negative, the number of occurrences of $C_A/< C_{Ai} >$ between the lower bound of $C_A/< C_{Ai} >$ and the sample mean occurred over a smaller range of $C_A/< C_{Ai} >$ than did the occurrences in the interval larger than the sample mean. Skewness was not observed when $\gamma_{\Delta E}$ was 0.01; even for cases in which $\gamma_{k0} = 0.10$ and $\gamma_{\Delta H}$ 0.10 the distributions were normal. When $\gamma_{\Delta E} = 0.01$, the minimum and maximum concentrations of $C_A/< C_{Ai} >$ were 0.00195 and 0.6897, respectively, representing more even smaller intervals below the sample mean.

Figure 4 shows the frequency distribution of T for a sample of 600 when $\gamma_{\Delta E}$ was 0.02. Observe that the frequency distribution is skewed far to right. Similar results were obtained when $\gamma_{\Delta E} = 0.01$, $\gamma_{k0} = 0.10$, and $\gamma_{\Delta H} = 0.10$. The reason for the skewed distribution of T when each of ΔE, k_0, or ΔH was random can be explained as follows. An analytical solution for T would be in the form of a sum of exponentials. Therefore, whatever the distribution of ΔE, k_0 or ΔH might be, the frequency distribution of T will tend to become some kind of exponential distribution skewed to the right.

The significance of these observations on the type of distributions of the reactor outputs is as follows. If $C_A/< C_{Ai} >$ can be assumed to be normally distributed for small $\gamma_{\Delta E}$ ($\leqq 0.01$), the tables of the standard normal distribution can be used to establish confidence limits for $C_A/< C_{Ai} >$. But if $\gamma_{\Delta E}$ is larger, and for T under certain circumstances, the standard normal tables will yield quite distorted confidence limits. One way to get the proper

confidence limits in these latter cases would be to run a large number of simulations, but considerable computer time would be used.

Sample Means and Sample Standard Deviations of $C_A/<C_{Ai}>$ and T

It is of interest for the purposes of design to know if the sample means of the reactor responses are different from the deterministic means and to see if the sample standard deviations of the responses are significantly affected by differences in the character of the distributions of the random inputs. The sample means of T in both the unsteady and the pseudo steady state were not significantly different (at $\alpha = 0.05$) from the corresponding deterministic solutions regardless of the types of random number generators used. In some instances the null hypothesis that the sample means of $C_A/< C_{Ai} >$ were the same as the deterministic solution was rejected (at $\alpha = 0.05$), but for practical engineering purposes the differences were not important and can be ignored.

The sample standard deviations of $C_A/< C_{Ai} >$ and T obtained when the uncorrelated random generators were used were not significantly different from each other, hence the assumptions about the type of distributions of the random inputs do not influence the dispersion of the responses.

If the propagation of error formula

$$\hat{\gamma}_{C_A/<C_{Ai}>} = \sqrt{\sum_j (\hat{\gamma}_{C_A/<C_{Ai}>})_j^2} \qquad (13)$$

where $(\hat{\gamma}_{C_A/<C_{Ai}>})_j$ represents the effect of a single coefficient of variation for variable or input j on $C_A/< C_{Ai} >$, is applied to compute the effect of dispersion on $C_A/< C_{Ai} >$ when several variables were simultaneously random, the computed coefficient of variation often did not differ significantly from the sample coefficient of variation obtained by simulation, and in most cases could be used for engineering design. For example, at a Peclet number of 4, the computed value of $\hat{\gamma}_{C_A/<C_{Ai}>}$ for the case in which k_0, ΔE, and T_w were simultaneously random (using the values of 0.1425, 0.3892, and 0.1542, obtained respectively, for the individual coefficients of variation) was 0.442 compared to a $\hat{\gamma}_{C_A/<C_{Ai}>}$ obtained by the Monte Carlo simulation of 0.468. $\hat{\gamma}_T$ when k_0, ΔE, and T_w were simultaneously random was 0.010, a value that agreed well with $\hat{\gamma}_T = 0.010$ obtained by the Monte Carlo simulation. The significance of these results is that a reasonably good approximation to the dispersion of the reactor responses can be obtained from just a few simulations representing the effect of individual random variables; a large number of simulations with all sorts of combinations of random variables is not required.

Relative Influence of the Random Variables on the Extent of Conversion

It is possible from the statistical analysis to learn which coefficient or input in a model has the most significant effect on the output variables, to decide which coefficients need to be measured most accurately, and to ascertain what input should be controlled more accurately. For the example reactor, when each of the coefficients and inputs individually was random, the parameters could be ordered in their effect on $\hat{\gamma}_{C_A/<C_{Ai}>}$ as follows (decreasing order):

(1) ΔE (2) T_w and k_0 (3) U and ΔH (4) v_z (5) $\tilde{D}_A$ (6) T_i (7) C_{Ai}

Therefore, small increase in $\gamma_{\Delta E}$ and γ_{T_w} could cause significant increases in $\hat{\gamma}_{C_A/<C_{Ai}>}$. The order of the effect of the parameters on $\hat{\gamma}_T$ was as follows:

(1) T_w (2) ΔE, U and v_z (3) ΔH (4) $\tilde{D}_A$, C_{Ai}, k_0 and T_i

Effect of Using an Autocorrelated Random Input

Real process inputs are likely to be correlated, and it is of interest to determine how the autocorrelation affects the conclusions presented so far. Two special cases were studied in which the input variables were autocorrelated in time:

Case (1): Each of C_{Ai}, T_w, and T_i was an autocorrelated random variable with the frequency of change of 10 changes per residence time.

Case (2): T_w was an autocorrelated random variable with a frequency of change of 10, and k_0 and ΔE were normal random variables.

As far as the frequency distributions of $C_A/< C_{Ai} >$ and T were concerned, the null hypothesis that they could each be represented by a normal distribution was tested and accepted. No significant differences were observed in the sample means, but the sample standard deviations were from 2 to 2½ times as large for the two cases as were the corresponding cases with uncorrelated variables. It was found that the remaining results for the two cases were essentially the same as those for the uncorrelated random inputs.

Application of the Results in Reactor Design

Confidence limits for the output variables $C_A/< C_{Ai} >$ and T can be calculated using the output sample standard deviations, and the confidence limits in turn can be used to compute the required overdesign factor based on known or assumed statistics of the random inputs and parameters. When calculated in this way, the overdesign factor becomes a quantitative safety factor in contrast to conventional deterministic design in which an arbitrary percentage based on past experience is added. It becomes possible for engineers to evaluate the physical and economic significance of safety factors in a quantitative way and to make more meaningful decisions in process design and operation.

The dispersion in the reactor responses at the exit can be used as follows. Figure 5 shows the sample means of $C_A/< C_{Ai} >$ in the pseudo steady state, the upper confidence limit for a confidence coefficient of $(1 - \alpha) = 0.95$, and the deterministic solution as a function of the rate factor for an ensemble Peclet number of 10. The coefficients and the inputs were all normal random variables each with a coefficient of variation and a frequency of change as previously indicated. The upper confidence limit was obtained by knowing that the frequency distribution of $C_A/< C_{Ai} >$ was represented by the normal probability density so that the standard tables could be employed.

Figure 5 can be interpreted as follows: If the ensemble Peclet number $< P > = < v_z > L/< \tilde{D}_A >$ is known to be 10 and if the ensemble rate factor $< R_1 > = < k_0 > L/< v_z >$ is known to be 3, $C_A/< C_{Ai} >$ has a deterministic value of 0.086 while the upper confidence limit of $C_A/< C_{Ai} >$ is 0.137 for a confidence coefficient of 0.95. The two curves can be used to compute an over-

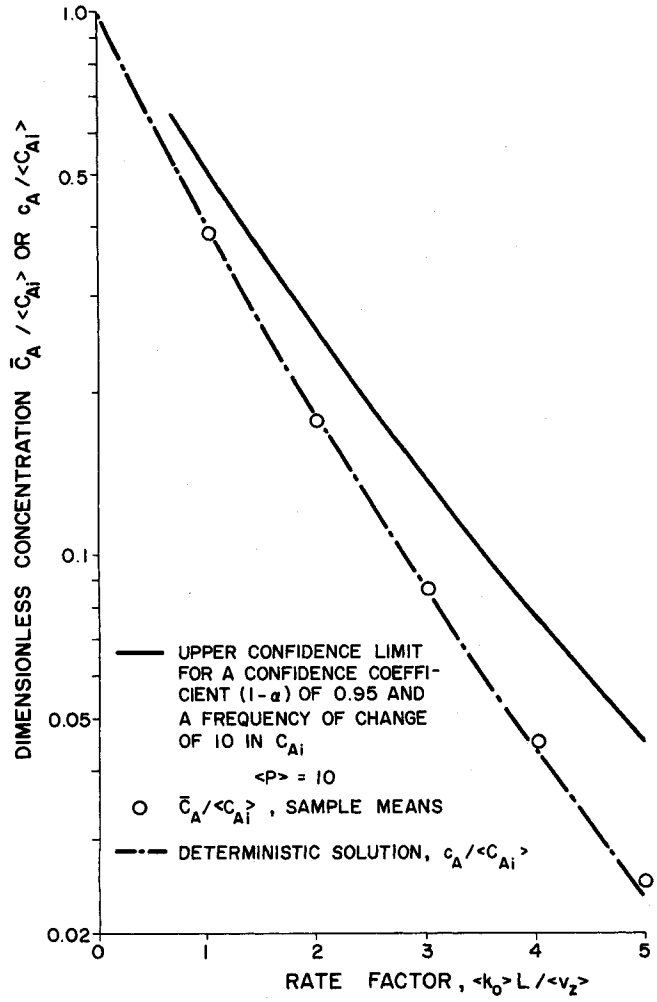

Fig. 5. Effect of simultaneously random $\tilde{D}_A$, k_0, v_z, and ΔE, ΔH, U, Tw, Ti, and C_{Ai} on the pseudo steady state response

design as follows. Suppose that $< P >$ is known or assumed to be 10 and that the desired conversion is 90%, that is, $c_A/< C_{Ai} > = 0.10$. Then $< k_0 > L/< v_z >$ is found to be 2.79 at $c_A/< C_{Ai} > = 0.10$ from the deterministic solution in Figure 5. An extension of $< C_A >/< C_{Ai} > = 0.10$ to the right to the upper confidence limit gives a value of $< k_0 > L/< v_z > = 3.53$. Therefore, the required overdesign factor is $3.53/2.79 = 1.27$, that is, the length of reactor should be increased by 27% to have a conversion of 90% for a confidence coefficient of 0.95. Overdesign factors can be computed for the other cases not shown in Figure 5 from the appropriate upper confidence limits given in the figures in Kado (1972).

A similar analysis can be carried out for the overdesign factor corresponding to a specified temperature. What we have not shown, but might be done, is the computation of the joint confidence region for the pair $(C_A/< C_{Ai} >, T)$ and use the joint confidence envelope to fix the overdesign factor at a given significance level.

NOTATION

C_A = concentration of reactant A, moles/volume
C_{Ai} = inlet concentration of a reactant A, moles/volume
C_p = molal heat capacity, energy/(moles) (Δ°)
$\tilde{D}_A$ = effective dispersion coefficient of component A in the axial direction, length²/time
E = expected value operator
ΔE = activation energy for chemical reaction, energy/moles
ΔH = heat of reaction, energy/mass
k_0 = reaction rate constant, $(\Delta°)^{-1}$
$\tilde{k}$ = effective thermal conductivity in axial direction, energy/(time) (length) (Δ°)
L = length of reactor
M = number of changes of fluid velocity per residence time
P = Peclet number, dimensionless
R_1 = rate factor $= \dfrac{< k_0 > L}{< v_z >}$
t = time
t^* = dimensionless time, $< v_z > t/L$
T = temperature
T_i = inlet temperature, °
T_w = wall temperature
r = radius of tubular reactor, length
R = gas law constant, energy/(moles) (Δ°)
u_z = forward fluid velocity, length/time
U = overall heat transfer coefficient at the wall, energy/(time) (length) (Δ°)
w_z = backward fluid velocity, length/time
v_z = fluid velocity, length/time
$\tilde{v}_z$ = averaged fluid velocity, length/time
z = axial distance, length
Z = random variable designated by subscript

Greek Letters

α = significance level
γ_X = ensemble coefficient of variation of X
$\hat{\gamma}_X$ = sample coefficient of variation of X
ρ = mass density, mass/volume

Subscripts

A = component A
i = inlet condition
0 = initial condition

Other

$< >$ = ensemble value
$\bar{\ }$ = as a bar overlay denotes sample average
$\hat{\ }$ = estimated value of variable

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