Some Important Considerations in Reactor Design

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Although much research effort has gone into the optimal control and the design of chemical reactors, there are still some important aspects of design which are sometimes overlooked. The purpose of this communication is to illustrate some of these and to show how they can influence the reactor design.

First let us look at the standard form of the reaction rate constant. Commonly the reaction rate constant is given by the Arrhenius expression

$$k = k_0 e^{-\frac{E}{RT}} \tag{1}$$

For example, Gaitonde and Douglas (*1*) used this expression for reactor design. The pre-exponential term in Equation (1) is very large and the exponential term is very small so that any small calculational error in the exponent could lead to serious errors.

Figure 1 shows that the estimate for the total cost of the reactor as considered by Gaitonde and Douglas [(*1*), case 1]* could be off by 20% merely by using the proper value for the gas constant R instead of the value 2.0 as has been apparently used by the authors. A more useful form for the reaction rate constant is

$$k = c\, e^{aT} \tag{2}$$

To obtain the constants c and a, we could evaluate k from Equation (1) for different values of T and plot the results as in Figure 2. The data in the temperature range of interest can be fitted by two straight lines to yield

$$k = \begin{cases} 0.849\, e^{0.099\Delta T}, & \Delta T \leq 0 \\ 0.849\, e^{0.091\Delta T}, & \Delta T > 0 \end{cases} \tag{3}$$

where

$$\Delta T = T - 620 \tag{4}$$

Here we have specified continuity at $T = 620$.

Equation (3) was tested with respect to Equation (1) and was found to give k within 4% of the value obtained by Equation (1) for the temperature range $583 \leq T \leq 652$ for the example under consideration. For design purposes Equation (3) is thus more than adequate for this 69° temperature range. However, Equation (3) is considerably easier to use than Equation (1).

The second important aspect of reactor design is to realize what really constitute the constraints for the system operation. When we consider Figure 1 in (*1*) which

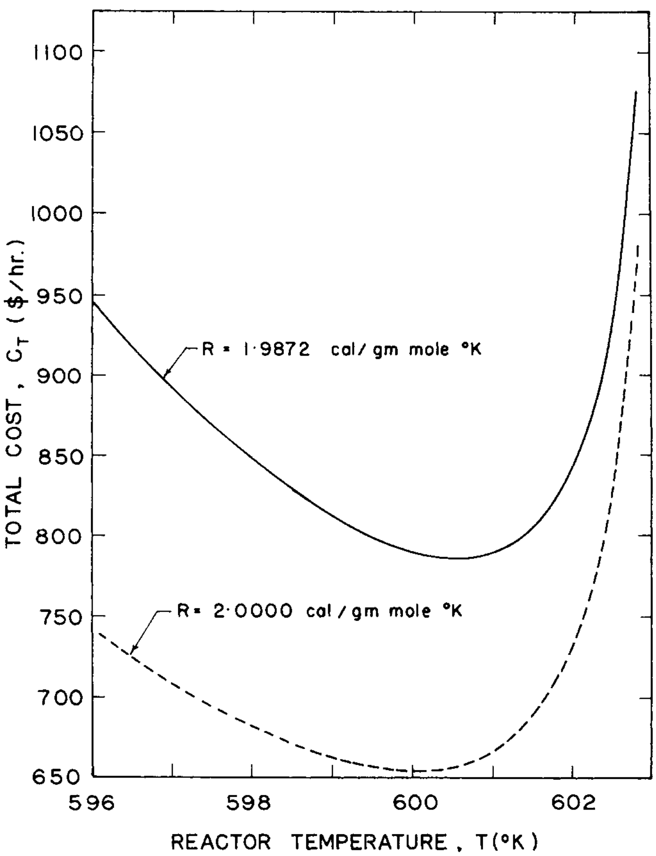

Fig. 1. Sensitivity of calculations on the value of R. Total cost versus reactor temperature as calculated from Equation (10) of Gaitonde and Douglas (*1*).

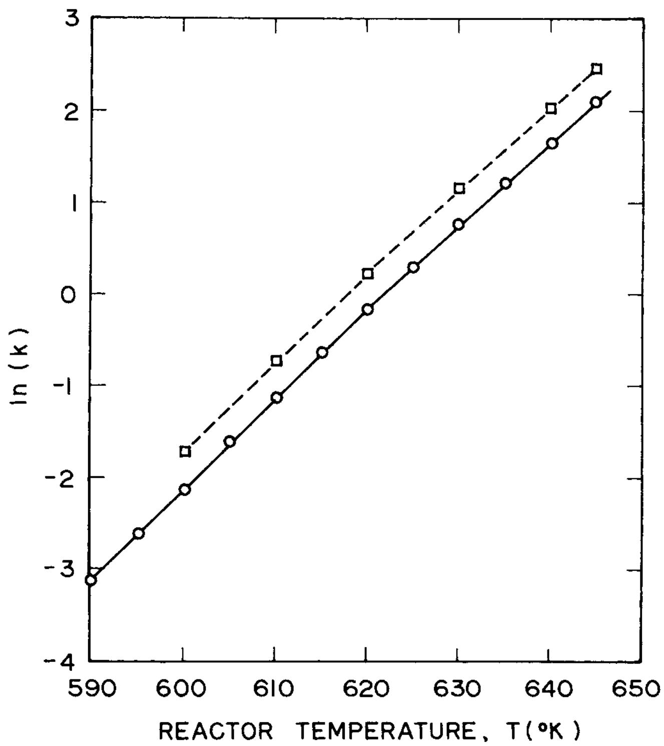

Fig. 2. *Ln(k)* versus reactor temperature, ○—○—○ calculations based on *R* = 1.9872 □—□—□ calculations based on *R* = 2.000.

* The numerical values given for Case 1 in Table 1 of (*1*) are used for Figures 1 and 2.

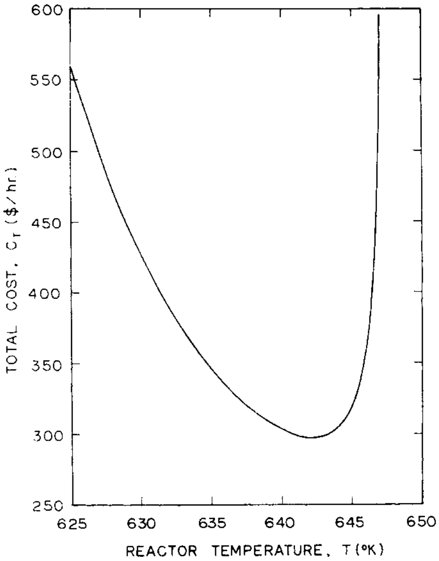

Fig. 3. Total cost versus reactor temperature with $T_H = 650°K$, $T_0 = 645°K$, $x = 0.000285$ gm.-mole/cu. cm., $R = 1.9872$ cal/gm.-mole °K. Rest of parameters same as in Case 1 of Gaitonde and Douglas (1).

corresponds to the dashed curve in Figure 1 in this communication, we observe a minimum. This minimum in the curve is caused by the choice of T_H and T_0. Since the inlet temperature of the heating fluid T_H does not have to be constrained at 606°K, we may perform a run in which we allow this constraint to be more relaxed. Figure 3 shows the result of such a run with $T_H = 650$, $T_0 = 645$, and $x = 0.000285$. The total cost C_T is reduced from 785 to 297; and the "operating cost" is reduced from 274 to 185. We can therefore increase the yield from 71.5% to 97.2% and also reduce the overall cost substantially by allowing the inlet temperature of the heating fluid to be increased.

Another important consideration is the means of operation and control. Using the same example, we realize at once that we have considerable freedom for choosing the means of supplying heat to the reactor and controlling the system. We are not limited to the use of a heating fluid; nor do we have to apply heat only to the reactor, for we may very well preheat the inlet stream.

These few fundamental considerations must be carefully examined before deciding how to operate and control the system. It is thus premature to state that by allowing the reactor to oscillate one obtains "a 5% lower operating cost than the optimum steady state plant" as is claimed by Heberling et al. (2).

LITERATURE CITED

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2. Heberling, P. V., N. Y. Gaitonde, and J. M. Douglas, *AIChE J.*, **17**, 1506 (1971).

Heat Transfer through a Wavy Film on a Vertical Surface

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Heat and mass transfer into and through liquid films occurs frequently in industrial process equipment. In most instances wave motion is encountered at the liquid-gas or liquid-vapor interface, and its presence probably explains why experimental measurements differ from theoretical predictions based on smooth laminar film flow. Experimental measurements show that wave motion intensifies heat and mass transport. This work is a computational investigation of heat transfer through wavy films.

The method by which vertical condensers are designed considers the resistance to heat transfer due to the condensate film which frequently is in transition flow. That the condensate is not in smooth film flow is treated by assuming the existence of turbulence and describing it by established eddy diffusivity methods (3). These design methods permit the analysis of heat transfer through the film for all condensate Reynolds numbers. An alternative description of the flow in the frequently encountered transition region would be laminar wavy flow.

Kapitza (7) presented an approximate analysis of heat transfer in periodic flows noting the effects that increase heat transfer. These are the decrease in the effective average film thickness due to the wave shape, an average film thickness less than the smooth film thickness for the same flow rate, and the convective effects of the periodic flow. Using the values of wave amplitude and film thinning from his film flow model, Kapitza estimated wavy film heat transfer to be 21% greater than that for the equivalent smooth film.

A generalized fluid mechanical model, based on the Kapitza model, has been assumed to describe heat transfer in wavy laminar film flows. The terminology is provided by Figure 1. Steady periodic wave motion is assumed with the surface shape described as a fluctuation about a constant value h_0

$$h = h_0(1 + \phi) \tag{1}$$

where ϕ is a function of $(x - ct)$. The x-component of

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