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The Co-current Reactor Heat Exchanger:

Part I. Theory

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Mathematical development is presented for the theory of a reactor heat exchanger in which the heat generated in the reaction stream is simultaneously transferred to a co-currently flowing coolant stream. The advantages of this scheme include isothermal conditions for the reaction stream, decreased parametric sensitivity, and improved stability.

SCOPE

Catalytic reactions which liberate (or absorb) large quantities of heat must have specially designed reactors to deal with them. Temperature excursions caused by insufficient cooling can lead to premature aging of the catalysts, production of undesirable side products, a shift of thermodynamic equilibrium against the completion of the reaction, or ultimately to the destruction of the reaction vessel. It is necessary to control the temperature deviations and to manage the temperature profile for the maximum yield of product. Numerous schemes have been employed (Froment, 1974).

This paper describes a theoretical analysis of a reactor heat exchanger that combines many of the desirable traits of current designs. Attainment of isothermal condition for reactant stream, parametric sensitivity, and stability of autothermal systems are considered.

CONCLUSIONS AND SIGNIFICANCE

The theory of a co-current reactor heat exchanger is presented and has led to the design of a reactor where the reaction stream remains isothermal in spite of highly exothermal reactions. It is shown that the isothermal design is easiest to obtain for first-order rate expressions and is extended to reactions of arbitrary order and to Langmuir-Hinshelwood kinetics. In each of these nonfirst-order cases, nonuniform catalyst distribution in the direction of flow is required.

An isothermal reactant stream is attained only at narrow windows of design and operation variables. These windows are defined by an exact balance between heat generation by exothermic reaction and heat removal by transport to the coolant stream. Outside of the window, the reactant stream either heats up or cools down.

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Autothermal processes are frequently operated under conditions of extreme sensitivity in regions where more than one steady state exists. One industrial example is that of the autothermal, countercurrent Haber-Bosch reactor (Baddour, 1965), where synthesis of ammonia is carried out in the region of multiple steady states. A co-current reactor heat exchanger operated autothermally is shown to be theoretically less sensitive to changes in the system parameters, compared to a similar countercurrent reactor heat exchanger. Moreover, the co-current reactor is shown here to be much more stable.

The optimal temperature profile in a fixed-bed reactor designed for highly exothermic reversible reactions is either uniform or slightly falling (Levenspiel, 1972). Four schemes are commonly used to attain a nearly flat reaction temperature profile. An inert, or a recycle of products, is often added to an inlet stream to lower the reactant concentration and to absorb the heat generated. Reactions are often carried out in a multiplicity of small diameter tubes bathed in a heat exchange medium such as boiling Dowtherm or molten salt. Fixed-bed reactors are frequently divided into stages with cooling by heat exchanges or by cold shots of reactants between stages. Finally, as in the Haber-Bosch reactor for ammonia synthesis (Froment, 1974), a heat exchanger is combined with a reactor so that heat generated along the reactor length is used to preheat a countercurrently flowing feed stream.

None of the above schemes operates with a precisely isothermal reactant unless catalyst dilution is used (Calderbank et al., 1968, 1969; Caldwell et al., 1969). When the Haber-Bosch reactor design is reversed by flowing the coolant concurrently, a constant reactant temperature can be attained.

If a fixed-bed reactor is to be designed so that the reactant remains isothermal, the rate of heat generation by the exothermal reaction must be exactly balanced by the rate of heat removal by transport to the coolant. For any isothermal reaction of positive order, the reaction rate falls as the reaction approaches equilibrium. Therefore, a more rapid cooling is needed at the reactant entrance than at the reactant exit. The countercurrent reactor heat exchanger cannot provide this, as the temperature difference between the reactant and the coolant is at a minimum at the reactant entrance, where the reaction rate and heat generation are at the maximum (see Figure 1). The co-current reactor heat exchanger, however, can be designed and tuned to match the heat generation and heat removal.

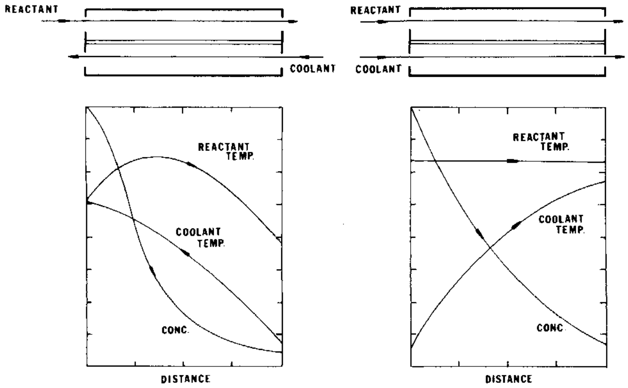

Fig. 1. Countercurrent and co-current reactor heat exchanger.

FIRST AND NTH-ORDER KINETICS

A co-current reactor heat exchanger can be modeled by a homogeneous model without axial or radical dispersions of heat or mass. The equations for heat and mass balances are

$$(v\rho C_p)^R \frac{dT^R}{dx} = k_\infty \exp\left(-\frac{E}{RT^R}\right) C^n(-\Delta H) - Ua(T^R - T^C) \quad (1)$$

$$(v\rho C_p)^C \frac{dT^C}{dx} = Ua(T^R - T^C) \quad (2)$$

$$u^R \frac{dC}{dx} = -k_\infty \exp\left(-\frac{E}{RT^R}\right) C^n \quad (3)$$

with boundary conditions

$$x = 0, \quad T^R = T^R{}_o \qquad T^C = T^C{}_o \qquad C = C_o \quad (4)$$

These equations can be rendered dimensionless as

$$\frac{d\theta^R}{d\xi} = -\mathrm{NTU}^R(\theta^R - \theta^C) + \beta Y^n \exp(-\alpha/\theta^R) \quad (1a)$$

$$\frac{d\theta^C}{d\xi} = \mathrm{NTU}^C(\theta^R - \theta^C) \quad (2a)$$

$$\frac{dY}{d\xi} = -\beta Y^n \exp(-\alpha/\theta^R) \quad (3a)$$

with boundary conditions

$$\theta^R = \theta^R{}_o; \quad \xi = 0 \qquad \theta^C = \theta^C{}_o; \quad \xi = 0 \qquad Y = 1; \quad \xi = 0 \quad (4a)$$

The number of transfer units on the reactants sides is $\mathrm{NTU}^R = Ual/(v\rho C_p)^R$, which is in general different from $\mathrm{NTU}^C = Ual/(v\rho C_p)^C$, since the flowing heat capacities of the two streams may be different.

The solution to Equation (2a) is

$$\theta^C = \theta^R{}_o - (\theta^R{}_o - \theta^C{}_o) \exp[-\mathrm{NTU}^C \cdot \xi] \quad (5)$$

The solution to Equation (3a) for constant θ^R is

$$Y = \exp[-\beta e^{-\alpha/\theta^R{}_o} \cdot \xi] \quad n = 1 \quad (6)$$

$$Y = [1 + (n-1)\beta e^{-\alpha/\theta^R{}_o} \cdot \xi]^{-1/(n-1)} \quad n \neq 1 \quad (6a)$$

For a first-order reaction, both the coolant temperature and the reactant concentration are exponential functions of distance. To be able to balance the heat transfer and heat generation of Equation (1), it is necessary and sufficient to specify that

$$\mathrm{NTU}^C = \beta e^{-\alpha/\theta^R{}_o} \quad (7)$$

and

$$\theta^R{}_o - \theta^C{}_o = \mathrm{NTU}^C/\mathrm{NTU}^R \quad (8)$$

to yield an exit concentration of

$$Y(1) = \exp[-\mathrm{NTU}^C] \tag{9}$$

For reactions other than first order, a uniform catalyst loading with a constant value of β would lead to a concentration profile that is the power function of Equation (6*a*), rather than the exponential function of Equation (6). This situation can be remedied by a nonuniform catalyst loading so that β is a function of ξ. To produce an exponentially declining heat generation profile with distance, it is necessary to load more catalyst near the exit for second-order reactions but to load more catalyst near the entrance for zero-order kinetics. The situation can also be remedied by a nonuniform reactor design so that Ua is a function of ξ.

The strategy of nonuniform catalyst loading can be attained by specifying

$$\beta = \frac{\mathrm{NTU}^R \exp(\alpha/\theta^{R_o} - \mathrm{NTU}^C\xi)}{[\exp(-\mathrm{NTU}^C\xi)]^n} \tag{10}$$

Let a pelleted catalyst of weight w be diluted with an inert solid (for example, quartz chips) to give a total weight W_T, and let the catalyst loading factor L be defined as w/W_T. If this loading factor is applied to Equation (10), the following relation is derived:

$$P = \frac{L_\xi}{L_{\xi=0}} = \exp[(n-1)\mathrm{NTU}^C\xi] \tag{11}$$

Here P is the ratio of the catalyst loading at any point in the reactor to the catalyst loading at $\xi = 0$.

LANGMUIR-HINSHELWOOD KINETICS

An example to which the isothermal condition can be attained is that of Langmuir-Hinshelwood kinetics (Boudart, 1968) in which the rate of reaction may be expressed in terms of dimensionless variables as

$$r(\theta^R, Y) = \frac{Co^2 k_\infty KaY}{CoKaY + 1} \exp(-\alpha/\theta^R) \tag{12}$$

If a derivation analogous to that for the first and n^{th}-order reactions is carried out for the Langmuir-Hinshelwood kinetics, the following equation for β results:

$$\beta = k\infty\tau^R = \left\{ \frac{\mathrm{NTU}^R \exp(-\mathrm{NTU}^C\xi + \alpha/\theta^R)}{Ka \exp(-\mathrm{NTU}^C\xi)} \right\} \times \quad Ka \exp(-\mathrm{NTU}^C\xi) + 1/Co) \tag{13}$$

The ratio of catalyst loading at any point in the reactor to the catalyst loading at $\xi = 0$ for the kinetics given by Equation (12) is

$$P = \frac{Ka \exp(-\mathrm{NTU}^C\xi) + 1/Co}{Ka + 1/Co} \tag{14}$$

GENERALIZED IRREVERSIBLE AND REVERSIBLE KINETICS

To generalize the isothermal criteria to any single rate expression, however complex, the following development is presented. Here, as in the preceding derivations, it is assumed that the rate of any catalytic reaction per unit volume of the reaction pass is directly proportional to the amount of catalyst present. For any single rate expression $r(\theta^R, Y)$, the mass balance in the reaction pass may be written as

$$\frac{dY}{d\xi} = \frac{-Lr(\theta^R, Y)\tau^R}{C_o} \tag{15}$$

Similarly, for the two heat balances

$$\frac{d\theta^R}{d\xi} = -\mathrm{NTU}^R(\theta^R - \theta^C) + \frac{Lr(\theta^R, Y)\tau^R}{C_o} \tag{16}$$

and

$$\frac{d\theta^C}{d\xi} = \mathrm{NTU}^C(\theta^R - \theta^C) \tag{17}$$

with the identical boundary conditions as given in Equation (4). Defining the fractional conversion Z as

$$Z \equiv 1 - Y$$

and integrating Equations (15), (16), and (17), we get

$$C_o \mathrm{NTU}^R[\theta^{R_o} - \theta^{C_o} - (\mathrm{NTU}^C/\mathrm{NTU}^R)Z] = Lr(\theta^R, Z)\tau^R \tag{18}$$

$$\xi = \frac{-1}{\mathrm{NTU}^C} \left\{ \ln\left[1 - \frac{\mathrm{NTU}^C}{(\theta^{R_o} - \theta^{C_o})\mathrm{NTU}^R} Z \right] \right\} \tag{19}$$

These two equations permit the catalyst distribution L to be derived as a function of length, once NTU^C, NTU^R, Z at $\xi = 1$, and $C_o\tau^R$ are set.

EXAMPLE

An example would serve to illustrate the application of the generalized development to an actual system. Consider the synthesis of methanol by the reaction

$$CO + 2H_2 \rightleftarrows CH_3OH$$

Calderbank (1969) has considered this process and has shown how to calculate the catalyst distribution to operate the reaction isothermally in a tubular reactor surrounded by a constant temperature heat exchange medium.

The kinetics and thermodynamic data are taken from the development of Natta (1955) for the synthesis of methanol over a ZnO-Cr_2O_3 catalyst, and from the data of Pasquon and Dente (1962) who concluded that the optimum reaction conditions in terms of yield are 395°C and 290 atm. Pasquon and Dente found the conversion of carbon monoxide at this point is 30 mole %, and that greater yields are not possible owing to the decomposition of the product, methanol, to methane and water at higher temperature. The rate expression, with the associated inlet conditions taken from the aforementioned references, is for 395°C and 290 atm:

$$r(\theta^R, Z) = \eta \frac{a_{CO}a_{H_2}{}^2 - a_{CH_3OH/Kp}}{(A + Ba_{CO} + Ca_{H_2} + Da_{CH_3OH})^3} \tag{20}$$

where

$A = 125$ $\qquad \eta = 0.67$
$B = 1.0$ $\qquad Kp = 2.67 \times 10^{-5}\ \mathrm{atm}^{-2}$
$C = 0.125$ $\qquad \Delta H = -24.45$ Kcal/g-mole
$D = 4.63$ $\qquad Cp = 7.6$ cal/g-mole
$\gamma_{CO} = 1$
$\gamma_{H_2} = 1$ $\qquad \Delta T_{AD} = 386°\mathrm{C}$
$\gamma_{CH_3OH} = 0.52$

with inlet molar percentages

$CO = 12\%$

$H_2 = 80\%$

Inerts = 8%

Let $1/\tau^R = 10\,000\ \mathrm{hr}^{-1}$ which is typical of industrial fixed-bed reactors, and let $(\theta^{R_o} - \theta^{C_o}) = 1$; that is,

Table 1. Methanol Synthesis Example

Conversion	Z	0	0.025	0.050	0.075	0.100	0.150	0.200	0.225	0.250	0.300
Catalyst loading	P	1	1.066	1.135	1.208	1.288	1.397	1.700	1.832	1.986	2.364
Distance	ϵ	0	0.071	0.144	0.218	0.295	0.455	0.615	0.714	0.806	1
Rate	$r(\theta^R, Z) \times 10^2$	17.38	15.34	14.60	13.34	12.17	10.06	8.20	7.37	6.58	5.16

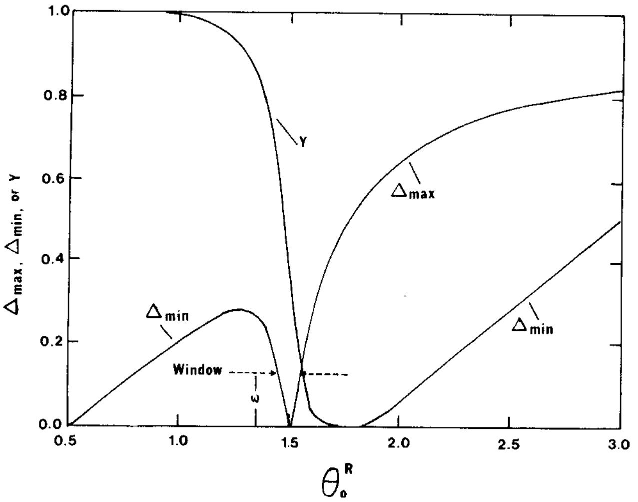

Fig. 2. Isothermal reaction produced by a narrow window in reactant inlet temperature. $\alpha = 11.11$, $\beta = 1\,620$, NTU $= 0.983$. Fraction remaining is Y, maximum and minimum temperature on reaction side is Δ_{max} and Δ_{min}, dimensionless inlet temperature is θ_0^R.

Table 2. Simulation Values

$\alpha = 11.111$
$\beta = 1620$
$NTU^C = 0.983$
$NTU^R = 0.983$
$\theta^C_o = 0.5$
$\theta^R_o =$ various

$T_o^C = 9$°C. For $NTU^C = NTU^R$, Equation (19) gives a value of 0.357 for NTU^C. Equation (18) can be solved for the ratio of the catalyst loading at any ξ to the loading at $\xi = 0$; that is

$$\frac{[(\theta^R{}_o - \theta^C{}_o - (NTU^C/NTU^R)Z(\xi)]}{[(\theta^R{}_o - \theta^C{}_o - (NTU^C/NTU^R)Z(0)]} = \frac{L(\xi)r[\theta^R{}_o, Z(\xi)]}{L(0)r[\theta^R{}_o, Z(0)]} \quad (21)$$

The catalyst distribution ratio P can be calculated as a function of $Z(\xi)$ after the reaction rate $r[\theta^R{}_o, Z(\xi)]$ is calculated for various values of $Z(\xi)$. These values of $Z(\xi)$ are then substituted into Equation (20) to relate $p(\xi)$ to ξ. Table 1 has been calculated using this procedure and the data of Pasquon and Dente. Isothermal operations can be attained at 30% conversion, while catalyst loading varies by somewhat more than a factor of two from entrance to exit.

WINDOWS OF ISOTHERMAL OPERATION

The reaction pass inlet temperature $\theta^R{}_o$ that gives an isothermal reaction pass profile is uniquely determined by NTU^C, NTU^R, the kinetic parameters α and β, and the coolant side inlet temperature $\theta^C{}_o$. If the reactant inlet temperature is changed while keeping the remaining parameters constant, the reactant temperature would not be constant and may go through a maximum or minimum temperature. Figure 2 shows this behavior for a first-order irreversible reaction.

The three curves shown on the figure are the fraction remaining, Y, the minimum temperature deviation defined

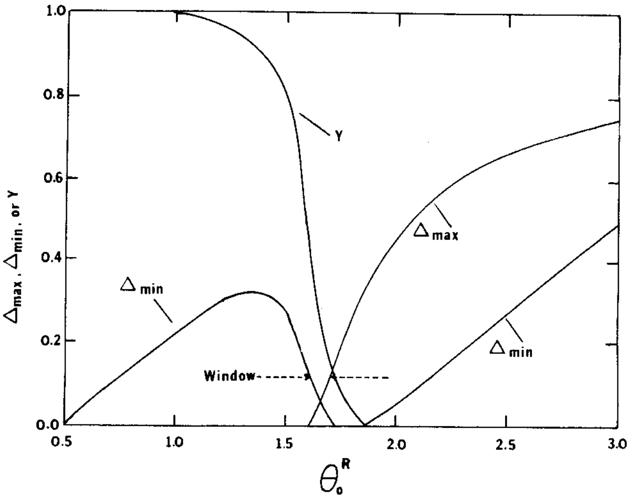

Fig. 3. The effect of increasing β to 2 500 on temperature window. Other parameter values as in Figure 2.

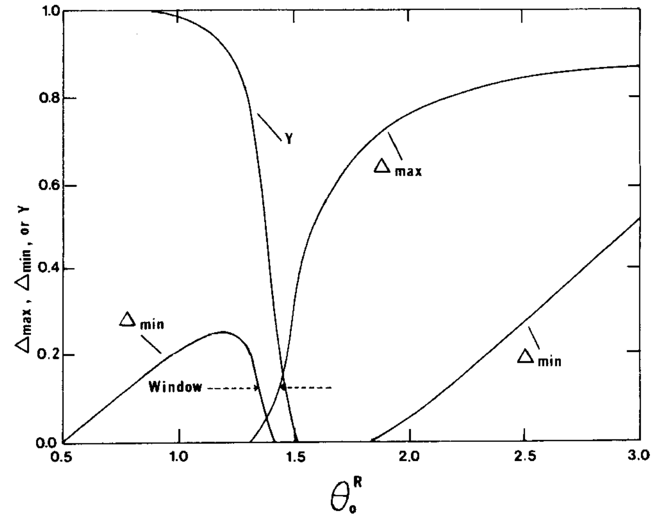

Fig. 4. The effect of decreasing β to 1 000 on temperature window. Other parameter values as in Figure 2.

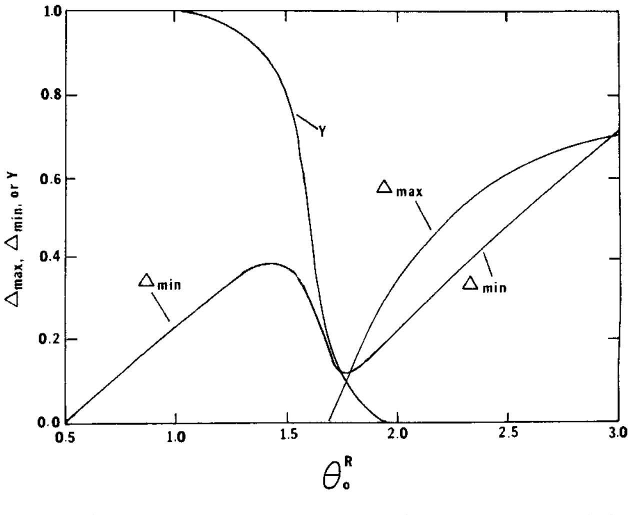

Fig. 5. The effect of increasing NTU to 2 on temperature window. Other parameter values as in Figure 2.

as

$$\Delta_{\min} = \frac{T^R{}_o - T^R{}_{\min}}{\Delta T_{AD}} = \theta^R{}_o - \theta^R{}_{\min} \qquad (22)$$

and the maximum temperature deviation defined as

$$\Delta_{\max} = \frac{T^R{}_{\max} - T^R{}_o}{\Delta T_{AD}} = \theta^R{}_{\max} - \theta^R{}_o \qquad (23)$$

where

$$\Delta T_{AD} = \left(\frac{-\Delta H C_o}{\rho C p}\right)$$

Values used in calculating Figure 2 are given in Table 2. At $\theta^R{}_o = 0.5$, the system is too cold, and conversion is negligible; there is also no heat transfer to coolant at $\theta^C = 0.5$. As $\theta^R{}_o$ increases, the $\Delta_{\min}$ curve first rises then falls. At $\theta^R{}_o = 1.0$, there is significant heat loss to the coolant, but conversion is still negligible. At higher values of $\theta^R{}_o$, conversion increases, and the minimum temperature increases until it equals the inlet temperature. At even higher values of $\theta^R{}_o$, a hot spot forms near the entrance of the reactant as the rate of reaction and heat release is more rapid than the rate of heat transfer. When all of the reactant is converted at very high values of $\theta^R{}_o$, the reaction stream becomes overcooled near the exit.

The most interesting feature of Figure 2 is the window formed by the $\Delta_{\max}$ and $\Delta_{\min}$ curves. If isothermality is defined as

$$|\theta^R{}_o - \theta^R(\xi)| < \epsilon \quad \text{for any } \xi \qquad (24)$$

The range over which $\theta^R{}_o$ may vary and still operate isothermally is defined on the left by the intersections of the $\Delta_{\max}$ and $\Delta_{\min}$ curves with $\Delta\theta = \epsilon$.

The shape of the window can assume other forms. For example, when β is increased from 1 620 to 2 500, increasing catalyst activity and residence time, the $\Delta_{\max}$ and $\Delta_{\min}$ curves move to the left and overlap as shown in Figure 3. Further increase of β would wipe out the isothermal window, since the reaction rate is fast and concentrates in a small area, so that the point where the $\Delta_{\min}$ and $\Delta_{\max}$ curves intersect eventually exceeds ϵ.

Decreasing β to 1 000 has a similar effect on the window shown in Figure 4. The $\Delta_{\max}$ and $\Delta_{\min}$ curves overlap and move to the right.

When either NTU^C or NTU^R is zero, the reaction pass is adiabatic, and no minimum temperature exists. The value of NTU is increased by larger heat transfer coefficient and slower flow rates. As the NTU's increase from zero to 0.983, isothermal conditions are attained. At the even higher values of NTU = 2.0, the system is too rapid in heat transfers. For any value of $\theta^R{}_o$, a minimum temperature curve having an S shape appears, shown in Figure 5. The window has vanished.

The conclusion of the above analysis is that a nearly isothermal reaction pass profile is obtainable for parameter values that deviate slightly from those specified by the isothermal criteria embodied in Equations (5) through (7). The precise deviation permitted in NTU^C, NTU^R, α, β, $\theta^R{}_o$, and $\theta^C{}_o$ depends on the size of a window described by the locus of maximum and minimum temperatures and an error bound ϵ which specifies the maximum temperature deviation allowable.

AUTOTHERMAL CO-CURRENT REACTOR HEAT EXCHANGERS

The co-current reactor heat exchanger can also be operated with or without additional input autothermally as shown in Figure 6. The term autothermal denotes that the heat of reaction alone is sufficient to maintain the elevated reaction temperature. If the coolant becomes

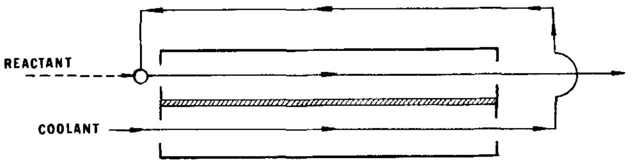

Fig. 6. Autothermal co-current reactor heat exchanger.

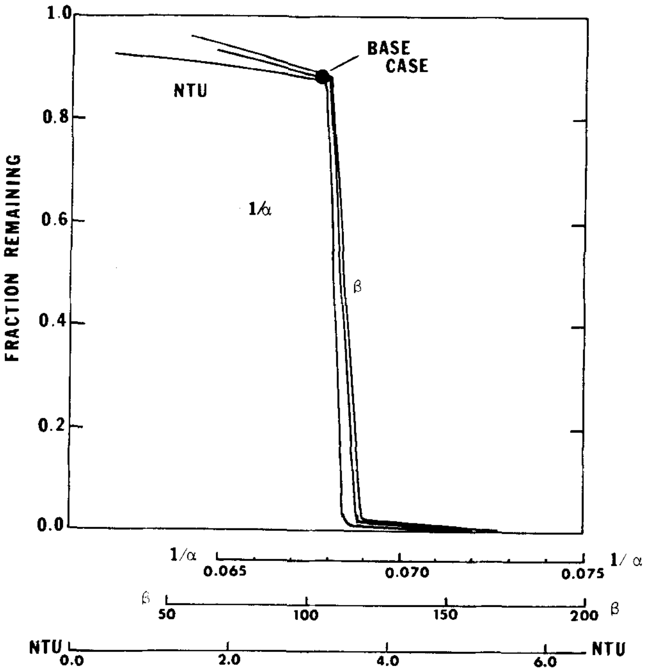

Fig. 7. Parameter sensitivity of fraction remaining in countercurrent reactor heat exchanger.

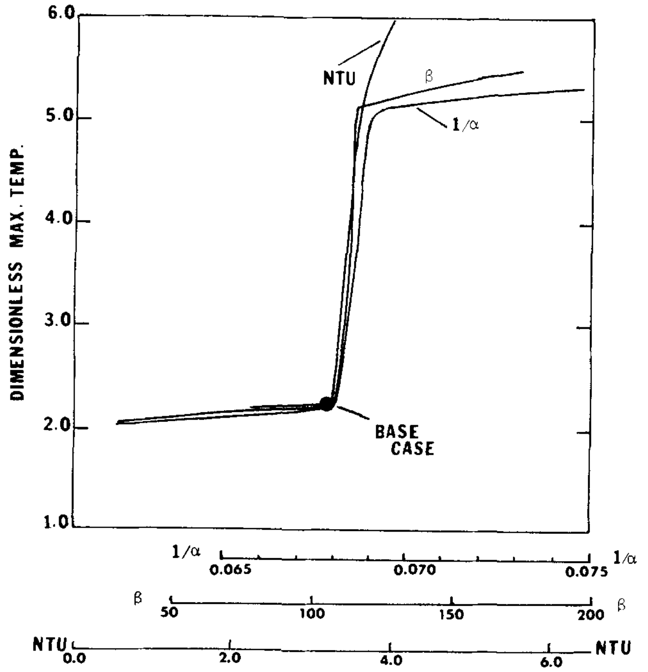

Fig. 8. Parameter sensitivity of maximum temperature in countercurrent reactor heat exchanger.

TABLE 3. BASE CASE FOR SENSITIVITY ANALYSIS

$NTU^R = NTU^C = 3.2$	$\beta = 107$
Need $\theta^R{}_o = 2.0$, $\theta^C{}_o = 1.9$	$\alpha = 0.068$

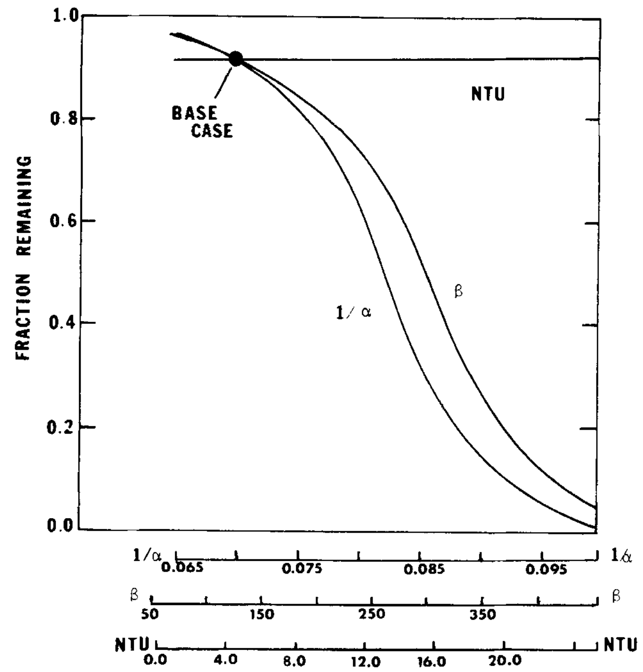

Fig. 9. Parameter sensitivity of fraction remaining in co-current reactor heat exchanger.

the reactant without additional inputs, the analyses developed earlier can be simplified by noting that

$$NTU^C = NTU^R \tag{25}$$

Autothermal reactors in which the coolant and reaction streams flow countercurrently have been shown to be very sensitive to parametric changes (Van Heerden, 1953, 1958; Baddour et al., 1965; Ampaya, 1975). Figures 7 and 8 show the effects of varying NTU, β, and $1/\alpha$ (or $R\Delta T_{AD}/E$) on the fraction converted and on the maximum temperature, respectively. The base case has been computed at a set of parameters about which the system shows extreme parametric sensitivity. These base conditions are given in Table 3. Note that small variations in either NTU, β, or α cause the system to extinguish or to light off rapidly.

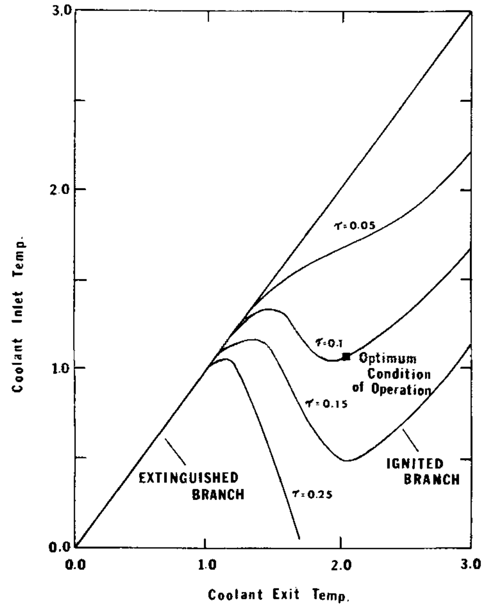

Fig. 11. The dependence of coolant exit temperature on coolant inlet temperature and residence time in seconds, for autothermal countercurrent reactor heat exchanger.

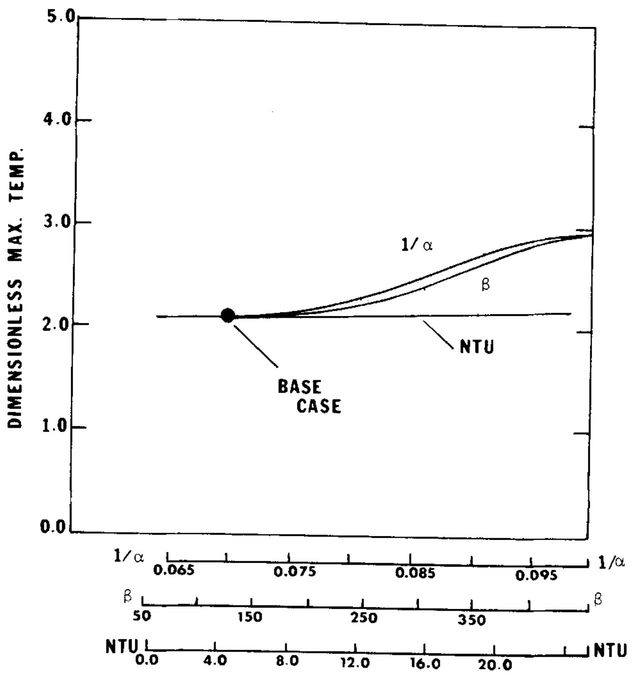

Fig. 10. Parameter sensitivity of maximum temperature in co-current reactor heat exchanger.

The effect of changing the same parameters about a base case having the same values as given in Table 3 for the autothermal concurrent case can be seen in Figures 9 and 10. Small variations in β or α have much less of an effect upon both the fraction converted and the maximum temperature than in the countercurrent case. Changing the NTU value has virtually no effect on either the fraction remaining or the maximum temperature in the concurrent case. Similar differences in sensitivity exist for other base case values.

STABILITY CONSIDERATIONS

The operation of autothermal reactors can be characterized by plotting the temperature of the stream entering the coolant pass vs. the temperature at the exit from the coolant pass (see, for example, Logeais, 1958). For

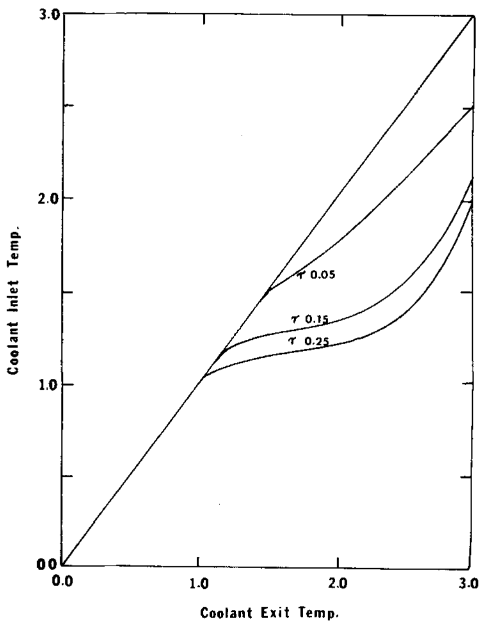

Fig. 12. The dependence of coolant exit temperature on coolant inlet temperature and residence time, for autothermal co-current reactor heat exchanger.

countercurrent autothermal reactors, it can be shown that there are often three exit temperatures corrresponding to the same inlet temperature (Van Heerden, 1953, 1958). Two of these three solutions to the steady state equations can be shown to be stable operating points, while the remaining operating point is unstable. This behavior is shown in Figure 11 in which the characteristic curves for various space times τ are plotted.

The right-hand part of the S shaped curves corresponds to the ignited or high conversion branch of operation. The left-hand branch of the curve corresponds to the extinguished section of the operating curve where coolant inlet temperature equals exit temperature. For reversible exothermic reactions, the optimum condition of operation is very near the minimum of the curves as shown on the $\tau = 0.1$ second curve. A small perturbation in inlet temperature may cause the reactor to blow out and move to the extinguished steady state.

Simulation of the autothermal cocurrent case results in the curves shown in Figure 12. No multiplicity is indicated for the three cases simulated. Simulation of longer space times shows that a region of steady state multiplicity does not exist for the co-current case. The co-current autothermal reactor is unconditionally stable.

CONCLUSIONS

A co-current reactor heat exchanger can be designed and operated with an isothermal reaction side profile. For first-order irreversible kinetics and a uniform catalyst loading, it is necessary to satisfy three distinct design equations:

$$\mathrm{NTU}^C = \beta \exp(-\alpha/\theta^R{}_o)$$

$$Y(1) = \exp\,(-\mathrm{NTU}^C)$$

$$(\theta^R{}_o - \theta^C{}_o) = \frac{\mathrm{NTU}^C}{\mathrm{NTU}^R}$$

For any other reaction order, the catalyst must be nonuniformly loaded to make the reaction behave as though the kinetics is first order, that is, exponential decay of concentration with distance.

The co-current reactor heat exchanger attains isothermal conditions only when all the design and operating variables are within narrow windows. The size of the window is determined by the maximum and minimum allowable deviation from isothermality.

The co-current reactor heat exchanger can also be operated as an autothermal reactor. The advantages of the co-current autothermal reactor over the conventional countercurrent autothermal reactor are a decrease in parametric sensitivity and an unconditional stability.

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NOTATION

a = heat transfer area to volume ratio, M^{-1}
C = concentration, $\mathrm{g/M^3}$ of reactor volume
Cp = heat capacity, J/g°K
E = activation energy, J/mole
Ka = adsorption coefficient
k_∞ = preexponential factor, 1/S
l = reactor length, M
L = catalyst loading factor, w/W_T
NTU = number of transfer units, $= Ual/\rho C_p V$
n = reaction order
p = catalyst loading factor in comparison to reactor inlet
$r(\theta^R, Y)$ = reaction rate, $\mathrm{g/M^3 \cdot S}$
T = temperature, °K
U = overall wall heat transfer coefficient, $\mathrm{J/°K\ M^2\ S}$
v = fluid velocity, M/S
W_T = total mass of material in reaction pass, g
w = mass of catalyst in reaction pass, g
x = distance along reactor, M, length
Y = fraction of reactant remaining, C/C_o
Z = fraction of reaction converted, $1 - C/C_o$

Greek Letters

α = activation parameter, $= (E/R\Delta T_{AD})$
β = activity parameter, $= (k_\infty \tau^R)$
γ = fugacity coefficient
Δ = deviation from isothermality
$-\Delta H$ = heat of reaction, J/mole
ΔT_{AD} = adiabatic temperature rise, $-\Delta H C_o/\rho_o Cp$, °K
ϵ = error parameter defined by Equation (25)
η = catalyst efficiency
θ = dimensionless temperature, $T/\Delta T_{AD}$
ξ = dimensionless length, x/l
ρ = density, $\mathrm{g/M^3}$
τ = space time, S, l/u^R

Superscripts

C = coolant pass
R = reactant pass

Subscripts

min = minimum value
max = maximum value
o = value at entrance

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