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Analysis and Design of Gas Flow Reactors with Applications to Hydrocarbon Pyrolysis

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The analysis and design of gas flow reactors are customarily based on a plug flow model. Because of transverse concentration and temperature gradients, however, kinetic constants and reactor lengths based on the plug flow model may be in gross error. This paper presents an approximate method of analysis which accounts for the effects of these gradients. We examine a gas in laminar flow which supports a first-order irreversible reaction. Compressibility effects are considered, and the diffusion fluxes are calculated with the full ternary diffusion equations. Instead of solving exactly the full equations of change which describe this system, the well-known Pohlhausen technique is adapted and approximate solutions which satisfy the integral forms of these equations are sought. This reduces the problem to the solution of a set of ordinary differential equations, which are integrated numerically. The main result is a set of graphs giving correction factors to be applied to plug flow kinetic constants and reactor lengths. Although primary interest is in hydrocarbon pyrolysis systems, the integral method graphs are applicable to other reaction systems.

Chemical engineers are often called upon to solve the two closely related problems: (1) Given conversion data obtained in a gas flow reactor, analyze the data to determine reaction rate constant. (2) Given reaction rate constants, design a gas flow reactor to obtain a specified conversion. We may call these, respectively, the analysis and design problems.

Hougen and Watson (*1*) presented solutions to these problems which were based on the assumption that the concentration profile was flat, the plug flow or one-dimensional model. Cleland and Wilhelm (*2*) considered the effect of a radial concentration gradient on a first-order reaction in an incompressible, isothermal fluid. The conservation equation for the reactant was integrated numerically. Later, Lauwerier (*3*) solved this problem analytically in terms of an infinite series of eigenfunctions.

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Numerical values calculated by Wissler and Schecter (*4*) showed excellent agreement with Cleland and Wilhelm's solution. Vignes and Trambouze (*5*) extended the solution to a second-order reaction system.

Nonisothermal systems have been studied by Gilbert (*6*) and by Chambré (*7*). Gilbert assumed the reactant concentration to be very low, so that the temperature field was due to heat transfer from the wall, and the thermal effect of the reaction was negligible. Chambré used a perturbation technique and obtained solutions valid at very low Damkohler numbers. To the approximation considered, it is found that if the fluid enters at the wall temperature, the temperature gradient vanishes and we have Lauwerier's isothermal solution.

These studies were based on the assumption of plug flow or well-developed incompressible flow. In both these cases the solution of the continuity and momentum equations to obtain the velocity profile is trivial. Recently, Ulrichson and Schmitz (*8*) studied a reaction in an isothermal incompressible fluid in the entrance region of a tubular reactor. Calculation of the velocity profile is, of course, no longer simple, but the assumption of constant physical properties means that the reaction has no effect on the hydrodynamic field. The axial and radial velocities are therefore determined as for a nonreacting flow, and they are then used in the conservation of species equation to calculate the extent of reaction as a function of tube length.

In the work cited above, Fick's law was used to calculate the diffusive flux, which is valid only for binary and multicomponent systems in which the binary diffusion coefficients are equal. In many multicomponent systems, the binary diffusion coefficients are not equal and Fick's law must be replaced by the multicomponent diffusion equations (*9*). Bird (*10*), Toor (*11*), and Hirschfelder (*12*) gave solutions for ternary diffusion through a stagnant film. Reinhardt (*13*) studied a dissociating ternary gas mixture in plug flow. By assuming the degree of dissociation to be small, he was able to linearize the equations and obtain solutions. Multicomponent diffusion in a fluid with a more interesting hydrodynamic field has been studied only by Prober (*14*), who solved the problem of mass transfer to a nonreacting multicomponent fluid in laminar boundary-layer flow.

In this paper we shall study the effects of transverse concentration and temperature gradients on a first-order reaction in a compressible fluid. Although we assume that the molal density is constant, we shall consider reactions in which moles are *not* conserved, so that the mass density is a function of the extent of reaction. This means that it will be necessary to solve simultaneously the continuity, momentum, energy, and conservation of species equations. This is the major difference between our work and earlier studies. The diffusive fluxes will be calculated using the multicomponent diffusion equations. To obtain solutions we will adapt the Pohlhausen technique of boundary-layer theory (*15*) and seek solutions which satisfy integral forms of the equations of change. This approach has previously been used by Kusik and Happel in a study of flow over catalyst particles (*16*). For internal flows it has been used in a study of natural convection by Lighthill (*17*), and in a study of compressible flow by Shang and Bloom (*18*).

BASIC EQUATIONS

Consider the steady laminar flow of an ideal gas which supports the first-order irreversible reaction

$$A = \nu B + \gamma C \tag{1}$$

We assume that the gas enters the reaction zone at the (constant) tube wall temperature T° with a well-developed parabolic velocity profile. The reaction has a reaction rate constant K and a heat of reaction h_r.

We consider two reactor geometries, a cylindrical tube, and an annulus. An annulus is not a particularly convenient geometry, but, if it is narrow, we may, in effect, unroll it and lay it flat, obtaining a two-dimensional channel as a result. We establish a coordinate system in which x measures the axial distance and y measures the transverse distance from the centerline.

In most cases of interest the tube or channel is slender, and we expect the axial velocity to be much larger than the transverse velocity and the axial gradients to be much smaller than the transverse gradients. In external flows these are just the conditions which lead to the boundary layer equations (*15*). We therefore feel intuitively, and a detailed order of magnitude analysis by Williams (*19*) has shown rigorously, that the conservation of momentum equations may be written in their boundary-layer form

$$\rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial y} = -\frac{\partial P}{\partial x} + \frac{\mu}{y^\epsilon} \frac{\partial}{\partial y}\left(y^\epsilon \frac{\partial u}{\partial y} \right) \tag{2}$$

$$\frac{\partial P}{\partial y} = 0 \tag{3}$$

In Equations (2) and (3) we have neglected gravitational forces. This is justified as long as natural convection currents are not induced. It is generally agreed (*20*) that in horizontal tubes natural convection is unimportant at Grashof numbers less than 1,000. For the systems studied here (cf. Table 2) the maximum Grashof number is of the order of 30. If the Grashof number is greater than 1,000, the analysis presented here is invalid. However, in those cases the mixing caused by the natural convection currents will reduce transverse temperature and concentration gradients, and the plug flow assumption will probably be valid.

Similarly, unless the Reynolds number is less than 2,100, the flow will be turbulent and our analysis is invalid. Here, too, the enhanced mixing will reduce transverse gradients, so that the plug flow assumption will probably be valid.

The remaining conservation equations are written exactly (*9*) without using the boundary-layer assumptions. We have the continuity equation

$$\frac{\partial}{\partial x}(\rho u) + \frac{1}{y^\epsilon}\frac{\partial}{\partial y}(y^\epsilon \rho u) = 0 \tag{4}$$

The conservation of species A and B

$$\frac{\partial}{\partial x}(\rho_A u) + \frac{1}{y^\epsilon}\left[\frac{\partial}{\partial y}(y^\epsilon \rho_A v) + \frac{\partial}{\partial y}(y^\epsilon j_{Ay})\right] = -K\rho_A \tag{5}$$

$$\frac{\partial}{\partial x}(\rho_B u) + \frac{1}{y^\epsilon}\left[\frac{\partial}{\partial y}(y^\epsilon \rho_B v) + \frac{\partial}{\partial y}(y^\epsilon j_{By})\right] = \nu K\rho_A \tag{6}$$

and, finally, the conservation of energy equation

$$c_p \frac{\partial}{\partial x}(\rho\, u\, T) + \frac{1}{y^\epsilon}\left\{ c_p \frac{\partial}{\partial y}(y^\epsilon \rho\, v\, T) + \frac{\partial}{\partial y}\left(y^\epsilon \sum_{i=1}^{3} j_{iy}\, c_{pi}\, T \right) \right\} = \frac{k}{y^\epsilon}\frac{\partial}{\partial y}\left(y^\epsilon \frac{\partial T}{\partial y}\right) - h_r K \rho_A \tag{7}$$

The only assumption involved in Equations (5), (6) and (7) are that in the axial direction, conduction of heat and mass is negligible compared with convection of heat and mass, and that the mass specific heat of the mixture is constant. To these equations we add the boundary conditions:

At $y = 0$ for all x, by symmetry

$$\frac{\partial u}{\partial y} = v = \frac{\partial T}{\partial y} = \frac{\partial \rho_i}{\partial y} = j_{iy} = 0; \; i = A, B, C \qquad (8)$$

At $y = w$ for all x, the wall conditions are

$$u = v = \frac{\partial \rho_i}{\partial y} = j_{iy} = 0; \; i = A, B, C \qquad (9a)$$

$$T = T^\circ \qquad (9b)$$

The initial conditions:

At $x = 0$ for all y

$$u = U\left(1 - \left(\frac{y}{w}\right)^2\right) \qquad (10a)$$

$$\rho_i = \rho_i^\circ, \quad i = A, B, C \qquad (10b)$$

$$T = T^\circ \qquad (10c)$$

We assume the reaction rate has the familiar Arrhenius dependence on temperature

$$K = F \exp\left(-E/Rg\,T\right) = K(T^\circ)\exp\left[\frac{-N_{Ea}\cdot(T^\circ - T)}{T^\circ}\right] \qquad (11)$$

Where $K(T^\circ)$ means K evaluated at T°. The equation of state is given by the ideal gas law. Since, however, variations in temperature and pressure will be moderate, the ideal gas law reduces to the specification that the molal density be constant.

The equations are put into dimensionless form by introducing the following transformation of variables:

$$\left.\begin{array}{l} \lambda = \dfrac{K(T^\circ)x}{U}; \; \eta = \dfrac{y}{w}; \\ u^+ = \dfrac{u}{U}; \; v^+ = \dfrac{v}{U}; \; P^+ = \dfrac{P}{\rho_o U^2}; \; T^+ = \dfrac{T^\circ - T}{T^\circ}; \\ \rho^+ = \dfrac{\rho}{\rho_o}; \; \rho_i^+ = \dfrac{\rho_i}{\rho_o}, \; j_{i\eta}^+ = \dfrac{j_{i\eta}}{\rho_o U}, \; i = A, B, C \\ \alpha = \dfrac{m_B}{m_A}; \; \beta = \dfrac{m_C}{m_A}; \; a = \dfrac{\mathcal{D}_{AC}}{\mathcal{D}_{AB}}; \; b = \dfrac{\mathcal{D}_{BC}}{\mathcal{D}_{AB}} \end{array}\right\} \qquad (12)$$

In terms of these variables our equations become

$$N_{Da}\,\rho^+ u^+ \frac{\partial u^+}{\partial \lambda} + \left(\frac{Uw}{\delta}\right)\rho^+ v^+ \frac{\partial u^+}{\partial \eta} = -N_{Da}\frac{dP^+}{d\lambda} + \frac{N_{Pr}}{\eta^\epsilon}\frac{\partial}{\partial \eta}\left(\eta^\epsilon \frac{\partial u^+}{\partial \eta}\right) \qquad (13)$$

$$\frac{dP^+}{d\eta} = 0 \qquad (14)$$

$$N_{Da}\frac{\partial}{\partial \lambda}(\rho^+ u^+) + \left(\frac{Uw}{\delta}\right)\frac{1}{\eta^\epsilon}\frac{\partial}{\partial \eta}(\eta^\epsilon \rho^+ v^+) = 0 \qquad (15)$$

$$N_{Da}\,\rho^+ u^+ \frac{\partial}{\partial \lambda}(x_A/\rho^+) + \left(\frac{Uw}{\delta}\right)\rho^+ v^+ \frac{\partial}{\partial \eta}\left(\frac{x_A}{\rho^+}\right) + \frac{N_{Pr}}{N_{Sc}\cdot\mathcal{D}_{AB}\eta^\epsilon}\frac{\partial}{\partial \eta}\left[\frac{\eta^\epsilon}{\rho^+}\left(\alpha D_{AB}\frac{\partial x_B}{\partial \eta} + \beta D_{AC}\frac{\partial x_C}{\partial \eta}\right)\right] = -N_{Da}\exp\left(\frac{-N_{Ea}\cdot T^+}{1 - T^+}\right)x_A \qquad (16)$$

$$N_{Da}\,\rho^+ u^+ \frac{\partial}{\partial \lambda}\left(\frac{x_B}{\rho^+}\right) + \left(\frac{Uw}{\delta}\right)\rho^+ v^+ \frac{\partial}{\partial \eta}\left(\frac{x_B}{\rho^+}\right) + \frac{N_{Pr}}{N_{Sc}\cdot\mathcal{D}_{AB}\eta^\epsilon}\frac{\partial}{\partial \eta}\left[\frac{\eta^\epsilon}{\rho^+}\left(D_{BA}\frac{\partial x_A}{\partial \eta} + \beta D_{BC}\frac{\partial x_C}{\partial \eta}\right)\right] = \nu\, N_{Da}\exp\left(\frac{-N_{Ea}\cdot T^+}{1 - T^+}\right)x_A \qquad (17)$$

$$N_{Da}\,\rho^+ u^+ \frac{\partial T^+}{\partial \lambda} + \left(\frac{Uw}{\delta}\right)\left\{\rho^+ v^+ + \frac{\sum_{i=1}^{3} c_{Pi}\, j_{i\eta}^+}{c_P}\right\}\frac{\partial T^+}{\partial \eta} = \frac{1}{\eta^\epsilon}\frac{\partial}{\partial \eta}\left(\eta^\epsilon \frac{\partial T^+}{\partial \eta}\right) + N_{Da}\cdot N_{Hr}\cdot\exp\left(\frac{-N_{Ea}\cdot T^+}{1 - T^+}\right)x_A \qquad (18)$$

In Equations (16) and (17), we have substituted the ternary diffusion equations (9) for $j_{A\eta}^+$ and $j_{B\eta}^+$. The boundary conditions become

At $\eta = 0$ for all λ

$$\frac{\partial u^+}{\partial \eta} = v^+ = \frac{\partial T^+}{\partial \eta} = \frac{\partial x_i}{\partial \eta} = j_{i\eta}^+ = 0; \; i = A, B, C \qquad (19)$$

At $\eta = 1$ for all λ

$$u^+ = v^+ = T^+ = \frac{\partial x_i}{\partial \eta} = j_{i\eta}^+ = 0; \; i = A, B, C \qquad (20)$$

At $\lambda = 0$ for all η

$$u^+ = 1 - \eta^2 \qquad (21a)$$

$$x_i = x_i^\circ, \; i = A, B, C \qquad (21b)$$

$$T^+ = 0 \qquad (21c)$$

We must now derive integral forms of Equations (13) to (18). This is done either by multiplying the equations by η^ϵ and integrating across the gap from $\eta = 0$ to $\eta = 1$, or simply by writing macroscopic balances across an element of thickness $d\lambda$. In either case, we derive the following five integral relations:

the continuity equation

$$\frac{d}{d\lambda}\int_0^1 \eta^\epsilon \rho^+ u^+ \, d\eta = 0 \qquad (22)$$

the conservation of momentum equation

$$\frac{d}{d\lambda}\int_0^1 \eta^\epsilon \rho^+ u^{+2}\, d\eta = -\frac{1}{\epsilon + 1}\frac{dP^+}{d\lambda} + \frac{N_{Pr}}{N_{Da}}\left.\frac{\partial u^+}{\partial \eta}\right|_{\eta=1} \qquad (23)$$

the conservation of species A

$$\frac{d}{d\lambda}\int_0^1 \eta^\epsilon x_A u^+ \, d\eta = -\int_0^1 \eta^\epsilon \exp\left(\frac{-N_{Ea}\cdot T^+}{1 - T^+}\right)x_A d\eta \qquad (24)$$

the conservation of species B

$$\frac{d}{d\lambda}\int_0^1 \eta^\epsilon x_B u^+ \, d\eta = \nu\int_0^1 \eta^\epsilon \exp\left(\frac{-N_{Ea}\cdot T^+}{1 - T^+}\right)x_A d\eta \qquad (25)$$

and the conservation of energy equation

$$\frac{d}{d\lambda}\int_0^1 \eta^\epsilon \rho^+ u^+ T^+ \, d\eta = \frac{1}{N_{Da}}\left.\frac{\partial T^+}{\partial \eta}\right|_{\eta=1} + N_{Hr}\int_0^1 \eta^\epsilon \exp\left(\frac{-N_{Ea}\cdot T^+}{1 - T^+}\right)x_A d\eta \qquad (26)$$

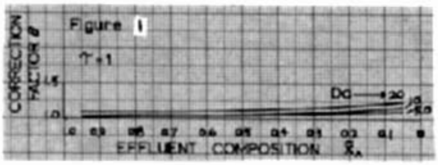

Fig. 1. Correction factor vs. effluent composition. Cylindrical tube, $N_{Hr} = 0$, $\tau = 1$.

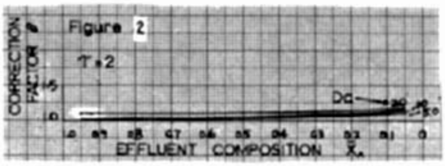

Fig. 2. Correction factor vs. effluent composition. Cylindrical tube, $N_{Hr} = 0$, $\tau = 2$.

REDUCTION TO ORDINARY DIFFERENTIAL EQUATIONS

Using Lighthill's method (*17*), we expand the dependent variables in even power series in η, with coefficients which are functions of λ. After satisfying boundary conditions (19) and (20) we find

$$u^+ = Z_1(\lambda)(1-\eta^2) + Z_2(\lambda)(\eta^4-\eta^2) + Z_3(\lambda)(\eta^6-\eta^2) \tag{27}$$

$$T^+ = Z_4(\lambda)(1-\eta^2) + Z_5(\lambda)(\eta^4-\eta^2) + Z_6(\lambda)(\eta^6-\eta^2) \tag{28}$$

$$x_A = Z_7(\lambda) + Z_8(\lambda)(\eta^2-\eta^4/2) + Z_9(\lambda)(\eta^6-3\eta^4/2) \tag{29}$$

$$x_B = Z_{10}(\lambda) + Z_{11}(\lambda)(\eta^2-\eta^4/2) + Z_{12}(\lambda)(\eta^6-3\eta^4/2) \tag{30}$$

These equations apply to both the two-dimensional channel ($\epsilon = 0$) and the cylindrical tube ($\epsilon = 1$). From this point on, however, the two cases must be treated separately. Since the procedure for both cases is similar, we will present only the analysis for the two-dimensional channel.

Substitution of Equations (27) and (29) into the integral conservation of A equation, (24), gives

$$\frac{d}{d\lambda}\int_0^1 \Big\{[Z_7 + Z_8(\eta^2-\eta^4/2) + Z_9(\eta^6-3\eta^4/2)] \times [Z_1(1-\eta^2) + Z_2(\eta^4-\eta^2) + Z_3(\eta^6-\eta^2)]\Big\}\, d\eta = -\int_0^1 \exp\left(\frac{-N_{Ea}\cdot T^+}{1-T^+}\right) x_A\, d\eta \tag{31}$$

Performing the indicated integration and differentiation on the left, we find

$$\left(\frac{2}{3}Z_7 + \frac{11}{105}Z_8 - \frac{17}{315}Z_9\right)Z_1' + \left(-\frac{2}{15}Z_7 - \frac{13}{315}Z_8 + \frac{19}{693}Z_9\right)Z_2' + \left(-\frac{4}{21}Z_7 - \frac{218}{3465}Z_8 + \frac{394}{9009}Z_9\right)Z_3' + \left(\frac{2}{3}Z_1 - \frac{2}{15}Z_2 - \frac{4}{21}Z_3\right)Z_7' + \left(\frac{11}{105}Z_1 - \frac{13}{315}Z_2 - \frac{218}{3465}Z_3\right)Z_8' + \left(-\frac{17}{315}Z_1 + \frac{19}{693}Z_2 - \frac{394}{9009}Z_3\right)Z_9' = -R \tag{32}$$

where we have set R, the average rate of reaction, equal to

$$R = \int_0^1 \eta^\epsilon x_A \exp\left(\frac{-N_{Ea}\cdot T^+}{1-T^+}\right) d\eta \tag{33}$$

It is understood that the integral is to be evaluated numerically. In Equation (32), and subsequent equations, a prime denotes differentiation with respect to λ. We write Equation (32) in the convenient form

$$a_{11}Z_1' + a_{12}Z_2' + a_{13}Z_3' + a_{17}Z_7' + a_{18}Z_8' + a_{19}Z_9' = b_1 \tag{34}$$

where the a_{1j} are the coefficients of Equation (32) and b_1 is the right side.

Similarly, we substitute Equations (27) to (30) into the four remaining integral conservation equations and obtain four more equations of the same form as Equation (34). We may write the set of five equations as

$$\sum_{j=1}^{12} a_{ij} Z_j' = b_i,\ i = 1, 2, 3, 4, 5 \tag{35}$$

In addition to the twelve unknowns, $Z_1, Z_2, \ldots, Z_{12}$, there is the additional unknown $dP^+/d\lambda$, for a total of thirteen. To the five equations (35), then, we must add eight new equations. These are obtained by satisfying the differential equations (13), (16), (17), and (18) at the centerline, $\eta = 0$, and at the wall, $\eta = 1$. For example, at $\eta = 1$, $u^+ = v^+ = 0$ and Equation (13) becomes

$$-\frac{dP^+}{d\lambda} + \frac{N_{Pr}}{N_{Da}}\frac{\partial^2 u^+}{\partial \eta^2} = 0$$

or with Equation (27)

$$-\frac{dP^+}{d\lambda} = \frac{N_{Pr}}{N_{Da}}(2Z_1 - 10Z_2 - 28Z_3) \tag{36}$$

which may be used to eliminate $dP^+/d\lambda$.

At $\eta = 0$, $v^+ = 0$ and Equation (13) becomes

$$\rho^+ u^+ \frac{\partial u^+}{\partial \lambda} = -\frac{dP^+}{d\lambda} + \frac{N_{Pr}}{N_{Da}}\frac{\partial^2 u^+}{\partial \eta^2}$$

or, with Equations (27) and (36)

$$C\, Z_1 Z_1' = \frac{N_{Pr}}{N_{Da}}(-12Z_2 - 30Z_3) \tag{37}$$

which is of the same form as Equation (34) and may be written

$$a_{61}Z_1' = b_6 \tag{38}$$

Similarly, satisfaction of (16), (17), and (18) at $\eta = 0$ gives three more equations of the same form. Our final three equations are obtained by satisfying Equations (16), (17), and (18) at $\eta = 1$. At $\eta = 1$, $u^+ = v^+ = 0$ and Equation (18) becomes

$$\frac{1}{N_{Da}}\frac{\partial^2 T^+}{\partial \eta^2} + N_{Hr}\cdot\exp\left(\frac{-N_{Ea}\cdot T^+}{1-T^+}\right) x_A = 0 \tag{39}$$

But here we have difficulty. The initial conditions (21*b*, *c*) indicate that $\partial^2 T^+/\partial \eta^2 = 0$, $\exp\left(\frac{-N_{Ea}\cdot T^+}{1-T^+}\right) = 1$, and $x_A = x_A^\circ$, values which do not satisfy Equation (39). This starting difficulty is not due to the boundary-layer technique. It is inherent in the equations and boundary

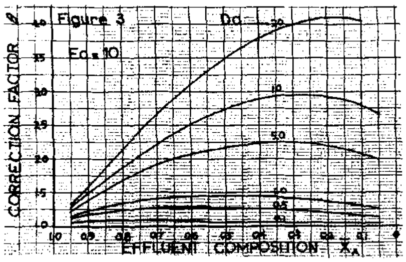

Fig. 3. Correction factor vs. effluent composition. Cylindrical tube, $N_{Hr} = 0.75$, $\tau = 1$, $N_{Ea} = 10$.

conditions and, in the final analysis, is because of the step change which we impose on the reaction rate constant at the plane $\lambda = 0$.

There are many ways to overcome this difficulty. We might, for example, modify the initial conditions to satisfy (39), but a simpler procedure is to replace the zero on the right of (39) by a forcing function $\psi(\lambda)$, which rapidly goes from the initial value of the left side of Equation (39) to zero; for example $\psi(\lambda) = N_{Hr} \cdot x_A{}^{o} \exp(-\xi\lambda)$. As ξ is increased, ψ approaches zero faster, and the error decreases, but the calculation time increases. We empirically determined the minimum value of ξ which would keep the error in the correction factor within acceptable limits by rerunning the same calculation with ξ equal to 1,000 and 10,000. Since the two calculations give almost identical correction factors, we use a value of $\xi = 1{,}000$ in all subsequent calculations. Finally, we note that instead of solving (39) as an algebraic equation, it is easier to differentiate it with respect to λ and to solve the resulting differential equation together with the set of differential equations we have already derived. Upon substituting Equations (27) to (30), we find

$$\frac{1}{N_{Da}}(-2Z_4' + 10Z_5' + 28Z_6') + N_{Hr}\left(Z_7' + \frac{1}{2}Z_8' - \frac{1}{2}Z_9'\right) = \psi' \qquad (40)$$

which is of the same form as Equation (34), and may be written

$$a_{10,4}Z_4' + a_{10,5}Z_5' + a_{10,6}Z_6' + a_{10,7}Z_7' + a_{10,8}Z_8' + a_{10,9}Z_9' = b_{10}$$

Similarly, satisfaction of (16) and (17) at $\eta = 1$ gives two more equations of the same form.

The twelve equations we have derived may be assembled into the one matrix equation

$$\overline{\overline{A}}\,\overline{Z'} = \overline{b} \qquad (41)$$

The initial conditions for (41) are obtained from the initial conditions on u^+ T^+ and x_i, Equations (21), through Equations (27) to (30). We find

$$\left.\begin{aligned} &\text{At } \lambda = 0 \\ &Z_1 = 1,\ Z_7 = x_A{}^{o},\ Z_{10} = x_B{}^{o} \\ &Z_2 = Z_3 = Z_4 = Z_5 = Z_6 = Z_8 = Z_9 = Z_{11} = Z_{12} = 0 \end{aligned}\right\} \qquad (42)$$

An analogous development of the equations describing flow in a cylindrical tube results in an equation of the same form as (41) with, of course, different definitions of the a_{ij}, and b_i, and the same initial conditions (42).

Fortran programs were written with the Gaussian elimination technique to solve Equation (41) and to integrate the differential equations with the Runge-Kutta method (*21*). We are able, therefore, to follow the evolution of $\overline{Z}$ with λ, and at suitable intervals to calculate the average concentration of A, $\overline{x_A}$, and the average temperature, $\overline{T^+}$

$$\overline{x_A} = \frac{\int_o^1 \eta^{\epsilon}\, x_A\, u^+\, d\eta}{\int_o^1 \eta^{\epsilon}\, u^+\, d\eta} \qquad (43)$$

$$\overline{T^+} = \frac{\int_o^1 \eta^{\epsilon}\, \rho^+ u^+\, T^+\, d\eta}{\int_o^1 \eta^{\epsilon}\, \rho^+ u^+\, d\eta} \qquad (44)$$

With $\overline{Z}$ known, it is possible to use Equation (36) to calculate $dP^+/d\lambda$ and, therefore, the pressure drop through the reactor.

ACCURACY OF THE INTEGRAL METHOD

We must first estimate the accuracy of the integral technique, and we will base that estimate on the accuracy of

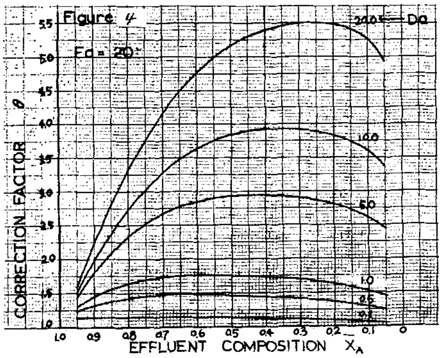

Fig. 4. Correction factor vs. effluent composition. Cylindrical tube, $N_{Hr} = 0.75$, $\tau = 1$, $N_{Ea} = 20$.

TABLE 1. COMPARISON OF EXACT AND APPROXIMATE CORRECTION FACTORS

Isothermal incompressible flow in a cylindrical tube

	Damkohler No. = ∞			Damkohler No. = 100			Damkohler No. = 10		
Avg. mole frac., $\overline{x_A}$	Cleland	Integral method	% Error	Cleland	Integral method	% Error	Cleland	Integral method	% Error
0.8	1.11	1.33	19.8	1.08	1.21	12.0	1.04	1.06	1.9
0.6	1.18	1.39	17.8	1.14	1.23	6.2	1.08	1.08	0.0
0.4	1.25	1.36	8.8	1.21	1.25	3.3	1.10	1.10	0.0
0.2	1.33	1.38	3.8	1.28	1.29	0.8	1.13	1.13	0.0

TABLE 2. CORRECTION FACTORS FOR LITERATURE DATA

Source	Run No.	Geometry	Reactant	Temp., °K.	Exit mole fraction, $\bar{x}_A$	N_{Sc}	N_{Ea}	N_{Hr}	N_{Da}	Correction factor
Silber (*22*)	98	Annulus $w = 0.0125$ in.	Propane	1,922	0.072	0.535	11.0	0.335	0.582	1.15
Silber (*22*)	91	Annulus $w = 0.0125$ in.	Propane	1,852	0.069	0.535	11.5	0.386	0.522	1.15
Silber (*22*)	75	Annulus $w = 0.0125$ in.	Propane	1,674	0.049	0.535	12.9	0.388	0.725	1.21
Silber (*22*)	51	Annulus $w = 0.0125$ in.	Propane	1,577	0.039	0.535	13.4	0.420	0.395	1.12
Silber (*22*)	52	Annulus $w = 0.0125$ in.	Propane	1,499	0.211	0.535	14.1	0.378	0.191	1.13
Silber (*22*)	38	Annulus $w = 0.0125$ in.	Propane	1,396	0.073	0.535	15.2	0.411	0.199	1.09
Sandler (*23*)	—	Cylinder $w = 0.256$ in.	*n*-Butane	973	0.500	0.380	23.2	0.436	0.270	1.19

Note: Prandtl number for all cases is 0.74.

the calculated correction factor θ. θ is defined as

$$\theta = \frac{K}{\hat{K}} = \frac{L}{\hat{L}} \qquad (45)$$

where K and L are the actual rate constant and reactor length, and $\hat{K}$ and $\hat{L}$ are the plug flow rate constant and reactor length. At any specified conversion, θ is calculated as

$$\theta = \lambda/\hat{\lambda} \qquad (46)$$

where λ is the actual dimensionless length required to achieve the specified conversion, and $\hat{\lambda}$ is the length based on the plug flow model. $\hat{\lambda}$ is calculated as

$$\sigma\hat{\lambda} = -\frac{(\tau - 1)\ (x_A^{\circ} - x_A)}{x_A(\tau - 1) + 1} + [1 + (\tau - 1)\ x_A^{\circ}] \ln \left[\frac{x_A(\tau - 1) + 1}{x_A(\tau - 1) + x_A/x_A^{\circ}} \right] \qquad (47)$$

where τ is the total number of moles of product per mole of reactant [$\tau = \nu + \gamma$ for reaction system (1)], and σ is a numerical constant equal to 2 for the cylindrical tube and 3/2 for the two-dimensional channel. Equation (41) may be obtained from equations given by Hougen and Watson (*1*).

Cleland's results for incompressible flow in a cylindrical tube were used to calculate correction factors as a function of effluent composition and Damkohler number. (Cleland's Damkohler number $N_{Da'}$ is based on mass diffusion and is related to our Damkohler number, which is based on conduction, through the equation, $N_{Da'} = N_{Sc} \cdot N_{Da}/N_{Pr}$.) These exact correction factors are compared with correction factors calculated with the integral method in Table 1. When the Damkohler number is reduced, the ratio of reaction rate to diffusion rate is also reduced; as a result the concentration profiles tend to flatten. We expect, therefore, that the power series approximation will be more accurate at lower Damkohler numbers, and this is shown in Table 1.

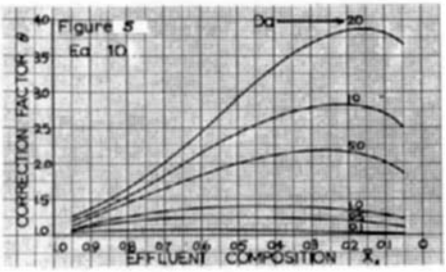

Fig. 5. Correction factor vs. effluent composition. Cylindrical tube, $N_{Hr} = 0.75$, $\tau = 2$, $N_{Ea} = 10$.

Although the comparisons in Table 1 are interesting, we really want to use the integral method in situations where no exact solutions exist, for example, nonisothermal, compressible flow, and we would like to have some estimate of the accuracy of the integral method under these conditions. Such estimates may be obtained as follows. Recall the power series equations, (27) to (30). We can consider each new term in the series as a correction to the existing terms. By solving a number of problems using one-, two-, and three-term power series, we can determine those regions in which the correction due to higher terms is negligible. Since the two parameters which have the strongest effect on the correction factor are the Damkohler number N_{Da} and the heat of reaction group N_{Hr}, the other parameters are held constant and the $N_{Da} - N_{Hr}$ plane is explored to determine the ranges of validity of the three power series solutions. A lower order power series is considered adequate if correction factors based on it agree with those calculated using a higher order series to within 3%. Of course, a four-term series solution would be necessary to fix exactly the upper limit on the range of validity of the three-term power series. However, it can be approximately fixed by assuming that each successive term added to the power series extends the range of validity by about the same amount. On this basis, for $N_{Hr} \leqq 0.75$, we are able to conclude that below a Damkohler number

TABLE 3. COMPARISON OF TERNARY AND BINARY CORRECTION FACTORS

Average mole fraction propane	Ternary system	Binary system	Percent error
0.8	2.04	2.03	0.5
0.6	3.86	3.75	2.7
0.4	5.23	4.96	5.1
0.2	5.56	5.24	6.0

Note: Both calculations based on $N_{Pr} = 0.74$, $N_{Hr} = 0.75$, and $N_{Ea} = 20$.

TABLE 4. INFLUENCE OF SCHMIDT AND PRANDTL NUMBERS ON CORRECT FACTORS

Damkohler No. = 10

Avg. mole frac., $\bar{x}_A$	Std. case $N_{Sc} = N_{Pr}$ = 0.74	$N_{Sc} = 0.2$ Corr. fac.	% Error	$N_{Sc} = 0.4$ Corr. fac.	% Error	$N_{Sc} = 0.6$ Corr. fac.	% Error	$N_{Sc} = 1.0$ Corr. fac.	% Error	$N_{Pr} = 0.85$ Corr. fac.	% Error
0.8	2.39	2.29	4.2	2.33	2.5	2.37	0.8	2.42	1.3	2.37	0.8
0.6	4.54	4.10	9.7	4.29	5.5	4.45	2.0	4.68	3.1	4.48	1.3
0.4	6.08	5.21	14.3	5.58	8.2	5.89	3.1	6.39	5.1	5.96	2.0
0.2	6.29	5.29	15.9	5.70	9.4	6.06	3.6	6.67	6.0	6.14	2.4

Damkohler No. = 5

Avg. mole frac., $\bar{x}_A$	Std. case $N_{Sc} = N_{Pr}$ = 0.74	$N_{Sc} = 0.2$ Corr. fac.	% Error	$N_{Sc} = 0.4$ Corr. fac.	% Error	$N_{Sc} = 0.6$ Corr. fac.	% Error	$N_{Sc} = 1.0$ Corr. fac.	% Error	$N_{Pr} = 0.85$ Corr. fac.	% Error
0.8	2.19	2.12	3.2	2.15	1.8	—	—	2.21	0.9	—	—
0.6	3.65	3.39	7.1	3.50	4.1	—	—	3.73	2.2	—	—
0.4	4.46	4.04	9.9	4.21	5.6	—	—	4.62	3.6	—	—
0.2	4.38	3.96	9.6	4.12	5.9	—	—	4.55	3.9	—	—

Note: All cases based on binary systems: $\tau = 2$, $N_{Ea} = 20$, $N_{Hr} = 0.75$.

of 10 for the two-dimensional channel and of 20 for the cylindrical tube, the integral method can be used to calculate correction factors with a maximum error of 3%.

EXAMINATION OF SPECIFIC CASES

Hydrocarbon pyrolysis data obtained in flow reactors are customarily analyzed on the basis of the plug flow model, Equation (47). To determine the errors which such an analysis introduces, some data obtained from the literature were reanalyzed with the integral method. The results are summarized in Table 2. In many of the cases listed in Table 2, the correction factor lies between 1.15 and 1.20, which indicates that analyses based on the plug flow model may introduce significant errors.

Since a plug flow analysis of kinetic data may lead to large errors, we would like to develop a generalized correction factor correlation which would eliminate the need to solve the full set of equations for each specific problem. Unfortunately, the large number of parameters which must be specified prohibits the presentation of a generalized correlation. We may hope, however, that a study of the equations will show that the correction factor is not very sensitive to variations in some of the parameters. These could then be held constant at assigned "standard" values and the dimensionality of the proposed generalized correlation reduced accordingly.

SIMPLIFICATIONS

Our treatment of a ternary system instead of a binary system introduces so many additional parameters (a, b, α, β, and ν) in place of only τ, that a mixing rule by which we could calculate an equivalent binary diffusion coefficient and, therefore, solve an equivalent binary problem in place of the full ternary problem would be useful. We construct a hypothetical experiment, modeled on Silber's (*22*) run 91, in which propane reacts according to

$$C_3H_8 = \frac{3}{2} C_2H_4 + H_2$$

However, to test the proposed mixing rule severely, we assume the Damkohler number to be 10, not 0.522 as it was in Silber's experiment. Under the conditions of the experiment, we find the following transport properties (*24*)

$$\mathcal{D}_{C_3\text{-}C_2} = 0.0236 \text{ sq.ft./sec.}, \quad \mathcal{D}_{C_3\text{-}H_2} = 0.105 \text{ sq.ft./sec.}$$

$$\mathcal{D}_{C_2\text{-}H_2} = 0.141 \text{ sq.ft./sec.}, \quad N_{Sc} = 0.535$$

We propose to calculate the equivalent binary diffusion coefficient as the stoichiometrically weighted average of the binary diffusion coefficients,

$$\mathcal{D}_{A\text{-Prod}} = \frac{\nu \mathcal{D}_{AB} + \gamma \mathcal{D}_{AC}}{\nu + \gamma} \tag{48}$$

For this case we find $\mathcal{D}_{C_3\text{-Prod}} = 0.0563$, and the Schmidt number based on this diffusion coefficient is 0.225. The ternary and binary correction factors are compared in Table 3.

We see that even at this high Damkohler number our simple mixing rule gives a maximum error of only 6%; therefore no attempt was made to investigate more complicated mixing rules. We may conclude, then, that it is not necessary to solve the full ternary equations, since

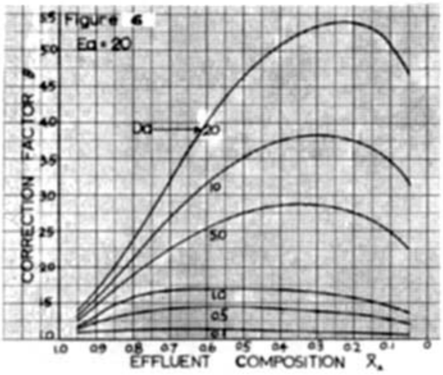

Fig. 6. Correction factor vs. effluent composition. Cylindrical tube, $N_{Hr} = 0.75$, $\tau = 2$, $N_{Ea} = 20$.

TABLE 5. INFLUENCE OF VELOCITY PROFILE ON CORRECTION FACTOR

Average mole fraction, $\bar{x}_A$	$N_{Da} = 10$, $N_{Hr} = 0.5$ Full equations	Modified equations	% Error	$N_{Da} = 10$, $N_{Hr} = 0.75$ Full equations	Modified equations	% Error
0.8	1.82	1.84	1.1	2.39	2.40	0.4
0.6	3.13	3.15	0.6	4.54	4.55	0.2
0.4	4.47	4.50	0.6	6.08	6.11	0.5
0.2	5.00	5.02	0.4	6.29	6.31	0.3

Note: Both calculations based on a binary system with $\tau = 2$, $N_{Pr} = N_{Sc} = 0.74$, and $N_{Ea} = 20$.

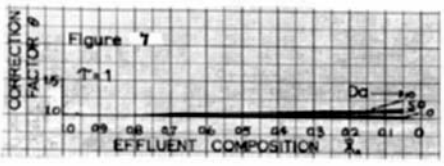

Fig. 7. Correction factor vs. effluent composition. Two-dimensional channel, $N_{Hr} = 0$, $\tau = 1$.

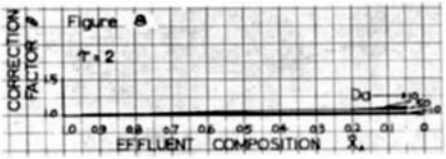

Fig. 8. Correction factor vs. effluent composition. Two-dimensional channel, $N_{Hr} = 0$, $\tau = 2$.

binary calculations, using Equation (48) to calculate effective binary diffusion coefficients, will give correction factors with sufficient accuracy. We will consider the binary reaction system

$$A = \tau B \tag{49}$$

The good agreement found above is related to another effect: the relatively small influence that variations in the Schmidt number have on the correction factors. The Schmidt number for self-diffusion of an ideal gas is approximately 0.75 (*9*). Based on our experience, as illustrated in Table 2 and in the example above, we believe that the Schmidt number of most hydrocarbon pyrolysis systems will lie between 0.2 and 1.0. In Table 4, correction factors calculated for a range of Schmidt numbers are compared with correction factors based on a standard value of Schmidt number, 0.74. We see that it is only for cases which have both a very low Schmidt number and a very high Damkohler number that the deviations from the standard case correction factors are significant; even for these cases the maximum error is only 16%.

We expect the correction factor to be more sensitive to variations in the Prandtl number, but here we are fortunate, since the expected range of the Prandtl number is quite narrow. Unfortunately, there does not seem to be any accurate method to calculate the thermal conductivity of polyatomic gases, although an equation proposed by Hirschfelder is widely used (*24*, *25*). This equation may be rewritten as

$$N_{Pr} = \frac{\tilde{c}_p}{1.33\,\tilde{c}_v + 0.431\,R_g} \tag{50}$$

Based on Equation (50) and some isolated data (*9*, *26*), it can be assumed that the Prandtl number of most hydrocarbon pyrolysis mixtures will lie between 0.74 and 0.85. Table 4 shows that within this range variations in the Prandtl number have a minor effect on the correction factor.

Finally we consider the effect of distortions of the parabolic velocity profile on the correction factor. Calcalculations are made in which the velocity profile is not permitted to distort, that is $Z_2$and Z_3 are kept at zero and the momentum equation is not satisfied. The centerline velocity Z_1 is allowed to vary in order to satisfy the integral continuity equation. The correction factors thus obtained are compared with those calculated with the full equations in Table 5. The agreement is excellent, and we conclude that accurate calculations of correction factors may be made without following the distortions of the velocity profile. We emphasize that it is distortions of the parabolic velocity profile which are negligible; if the density changes the centerline velocity must be allowed to vary in order to satisfy the continuity equation.

GENERALIZED CORRELATION

The simplifications discussed above indicate that we may confine our attention to binary systems and, therefore, replace the parameters α, β, ν, a, and b, with the single parameter τ, and that we may set the Prandtl and Schmidt numbers at their standard value, 0.74. (The third simplification, that Z_2 and Z_3 may be set identically to zero, was not discovered until after these calculations were made.) Correction factors calculated on this basis should be applicable to all hydrocarbon pyrolysis systems, except those which have both a very low Schmidt number (less than 0.4) and a very high Damkohler number (greater than 5). Even for these exceptional systems the maximum error in the correction factor will be only 16%; for average systems the maximum error in the correction factor will be about 6%.

We have, then, to consider only the four parameters, τ, N_{Hr}, N_{Ea}, and N_{Da} and, of course, reactor geometry, cylindrical tube, and two-dimensional channel. By considering the values likely to be encountered in hydrocarbon pyrolysis systems, and also keeping in mind the range of validity of our equations, we assigned the following values to the parameters: $\tau = 1$,* 2; $N_{Hr} = 0, 0.25, 0.50, 0.75$; $N_{Ea} = 10, 20$; $N_{Da} = 0.1, 0.5, 1, 5, 10, 20$ (for cylindrical tube); and $N_{Da} = 0.05, 0.1, 0.5, 1, 5, 10$ (for two dimensional channel).

All possible combinations of these parameters are used in a series of calculations covering both the cylindrical tube and the two-dimensional channel. Part of the results are presented as graphs of correction factor vs effluent composition in Figures 1 to 12.† These graphs show that correction factors of two, three, and even higher are not uncommon, indicating that an analysis based on the plug flow model may lead to gross errors. On the other hand, sufficient conditions for the correction factor to be negligible are that N_{Hr} be less than 0.25 and N_{Da} be less than

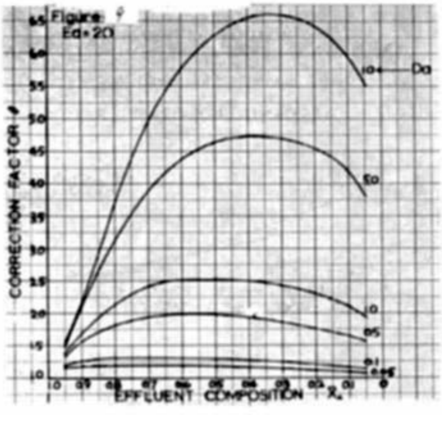

Fig. 9. Correction factor vs. effluent composition. Two-dimensional channel, $N_{Hr} = 0.75$, $\tau = 1$, $N_{Ea} = 10$.

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* Note that with our assumption of constant molal density $\tau = 1$ corresponds to incompressible flow. In fact, the correction factors presented in Figure 1 for $N_{Hr} = 0$, $\tau = 1$ are those which are tabulated in Table 1.

† Figures 13 to 28 and Table 6 have been deposited as document 8543 with the American Documentation Institute, Photoduplication Service, Library of Congress, Washington 25, D. C., and may be obtained for $3.75 for photoprints or $2.00 for 35-mm. microfilm.

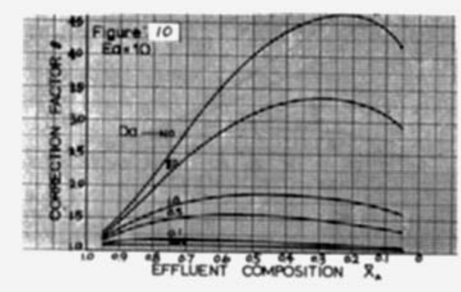

Fig. 10. Correction factor vs. effluent composition. Two-dimensional channel, $N_{Hr} = 0.75$, $\tau = 1$, $N_{Ea} = 20$.

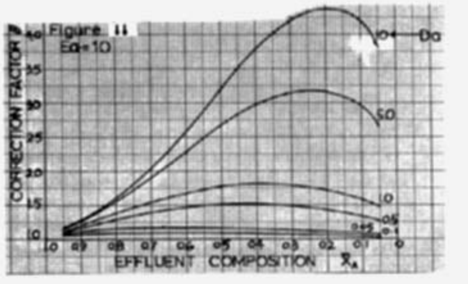

Fig. 11. Correction factor vs. effluent composition. Two-dimensional channel, $N_{Hr} = 0.75$, $\tau = 2$, $N_{Ea} = 10$.

0.10 for the cylindrical tube or less than 0.05 for the two-dimensional channel.

The relatively small correction factors calculated for the cases were $N_{Hr} = 0$. Figures 1, 2, 7, and 8 show that the effects of temperature gradients are far more important than the effects of concentration gradients. An interesting fact revealed by a study of Figures 1 to 12 is that the correction factor is not too sensitive to τ. (This is not to say that rate constants and reactor lengths are not sensitive to variations in τ; Equation (47) shows that they are. We are discussing here the sensitivity of the correction factor only.) The maximum difference between correction factors for $\tau = 1$ and $\tau = 2$ is about 40%, but this is an extreme case, and in general the difference is about 5 to 20%. Therefore, not only are we able to interpolate to obtain correction factors for values of between one and two, but we may also extrapolate to get correction factors for values of τ somewhat greater than two.

The use of Figures 1 to 12 is demonstrated by the following illustration. Consider a hypothetical experiment for which we have the following data:

Reactor geometry	Two-dimensional channel
τ	2
N_{Hr}	0.75
N_{Ea}	20.0
Effluent composition, $\bar{x}_A$	0.30

We wish to calculate the reaction rate constant. The first step is to calculate the rate constant with the plug flow equation (47). Assume this has been done and that the Damkohler number based on the plug flow rate constant is 0.50. We must use Figure 12 in a trial and error calculation to determine the correction factor. We find the correct Damkohler number to be 1.23. The kinetic constants are in the same ratio as the Damkohler numbers

$$\frac{K}{\hat{K}} = \frac{Da}{\hat{Da}} = \frac{1.23}{0.50} = 2.46$$

The actual rate constant is then 2.46 times the one-dimensional rate constant.

The design problem is more straightforward, since in this case the rate constant and the Damkohler number are known. One begins by using the plug flow equation (47) to calculate the reactor length. Then, with the Damkohler number known, the appropriate graph is entered and the correction factor read. The actual reactor length is obtained by multiplying the plug flow length by the correction factor.

CONCLUSIONS AND RECOMMENDATIONS

We have shown that the plug flow assumption is valid only if N_{Hr} is less than 0.25 and N_{Da} is less than 0.10 for the cylindrical tube or less than 0.05 for the two-dimensional channel. Under other conditions the effects of transverse temperature and concentration gradients are significant and must be accounted for.

We have also shown that the integral method is a simple and, in its range of validity, an accurate method of computing correction factors to be applied to plug flow kinetic constants and reactor lengths. The range of validity of the integral method is established precisely by comparing its results with exact solutions whenever possible and, more importantly, by comparing correction factors computed on the basis of one-, two-, and three-term power series.

Although we have been primarily interested in hydrocarbon pyrolysis systems, the integral method is general and may be applied to any reacting system, provided the flow is laminar and natural convection effects are absent. Indeed, our main results (Figures 1 to 12) apply to any system which meets these conditions and whose transport and thermodynamic properties fall in the range covered by the graphs.

We also presented data which support three useful simplifications: (1) within their normal range, variations of the Schmidt and Prandtl numbers have only a minor effect on the correction factor; (2) a full treatment of ternary diffusion is unnecessary, since calculations based on Fick's law, using Equation (48) to calculate equivalent binary diffusion coefficients, give correction factors with sufficient accuracy; (3) it is not necessary to follow the distortions of the velocity profile since they have a minor effect on the correction factor. Simplifications (1) and (2) allow us to reduce the dimensionality of the generalized correlation, while simplifications (2) and especially (3) enormously reduce the complexity of the integral method.

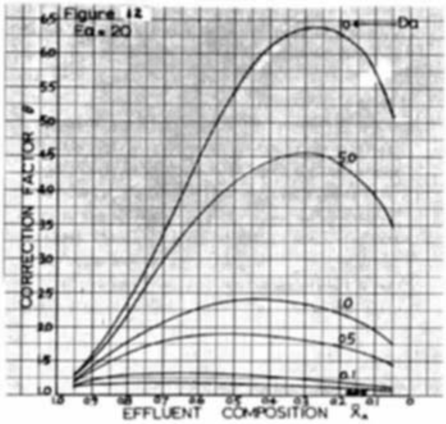

Fig. 12. Correction factor vs. effluent composition. Two-dimensional channel, $N_{Hr} = 0.75$, $\tau = 2$, $N_{Ea} = 20$.

With this reduction in complexity, the integral method may be used to study systems undergoing more complex chemical reactions, for example, consecutive, simultaneous or reversible reactions, and reactions with orders other than first. None of these modifications would affect the basic structure of the problem, as given by Equation (41); they would only make the calculation of $\overline{b}$ more complicated.

ACKNOWLEDGMENT

We would like to thank the National Science Foundation for a Cooperative Fellowship awarded to M.L.T. The calculations reported here were made at the AEC Computing Center at the Courant Institute of Mathematical Sciences.

NOTATION

a = transport parameter, defined in Equation (12), dimensionless
a_{ij} = coefficients in matrix $\overline{\overline{A}}$ of Equation (41)
b = transport parameter, defined in Equation (12), dimensionless
b_j = coefficients in vector $\overline{b}$ of Equation (41)
C = $Z_7(1-\beta) + Z_{10}(\alpha-\beta) + \beta_1$, dimensionless
c_p = heat capacity at constant pressure, per unit mass, L^2/t^2T
$\tilde{c}_p$ = heat capacity at constant pressure, per unit mole, ML^2/t^2T mole
D_{ij} = multicomponent diffusion coefficient for i in j, L^2/t
$\mathcal{D}_{ij}$ = binary diffusion coefficient for system $i - j$, L^2/t
E = activation energy, ML^2/t^2
F = frequency factor, t^{-1}
h_r = heat of reaction per unit mass A consumed, L^2/t^2
j_{iy} = mass flux of species i in y direction relative to mass average velocity, M/tL^2
K = reaction rate constant, t^{-1}
k = thermal conductivity, ML/t^3T
L = reactor length, L
M = mass
m_i = molecular weight of species i, M/mole
N_{Da} = Damkohler number, $K(T^\circ)w^2/\delta$, dimensionless
$N_{Da'}$ = Damkohler number, $K(T^\circ)w^2/\mathcal{D}_{AB}$, dimensionless
N_{Ea} = activation energy group, E/R_gT°, dimensionless
N_{Hr} = heat of reaction group, h_r/c_pT°, dimensionless
N_{Pr} = Prandtl number, $c_p\mu/k$, dimensionless
N_{Sc} = Schmidt number, $\mu/\rho_o\mathcal{D}_{AB}$, dimensionless
P = static pressure, M/Lt^2
R_g = gas constant, ML^2/t^2T mole
R = average dimensionless rate of reaction, defined in Equation (33)
T = absolute temperature, T
t = time
u = x component of velocity, L/t
v = y component of velocity, L/t
w = reactor radius or half width of annulus, L
x = axial coordinate, L
x_i = mole fraction of species i, dimensionless
x_i = average mole fraction of species i, dimensionless
y = transverse coordinate, L
U = centerline velocity, L/t
Z_j = functions of λ, defined in Equations (27) to (30)

Greek Letters

α = stoichiometric parameter, defined in Equation (12), dimensionless
β = stoichiometric parameter, defined in Equation (12), dimensionless
γ = stoichiometric coefficient, defined in Equation (1), dimensionless
δ = thermal diffusivity, k/ρ_oc_p, L^2/t
ϵ = coefficient, $\epsilon = 0$ for two-dimensional channel, $\epsilon = 1$ for cylindrical tube, dimensionless
η = dimensionless transverse coordinate, defined in Equation (12)
θ = correction factor, defined in Equation (45), dimensionless
λ = dimensionless axial coordinate, defined in Equation (12)
μ = viscosity, M/Lt
ν = stoichiometric coefficient, defined in Equation (1), dimensionless
ρ = density, M/L^3
ρ_o = density of A at prevailing temperature and pressure, M/L^3
τ = stoichiometric coefficient, defined in Equation (49), dimensionless

Superscripts

$\wedge$ = based on plug flow model
$+$ = dimensionless variable, defined in Equation (12)
o = initial condition

Subscripts

A, B, C = species A, B, and C

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