COMMUNICATIONS TO THE EDITOR

Some Aspects of Isothermal Laminar Flow Reactors

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Exact solutions to the diffusion equation neglecting axial diffusion were determined for first-order reversible homogeneous reaction in a fully developed laminar flow between infinite parallel plates with heterogeneous reaction occurring simultaneously at the catalytic walls. These solutions were extended to the case of mass transfer from constant concentration walls to laminar flowing fluid with homogeneous reaction in the flow. The effect of axial diffusion was considered and found to be small except for very slow flows, wherein buoyancy effects invalidate the parabolic velocity distribution.

Recently, solutions for homogeneous first-order chemical reaction in tubular reactors under isothermal conditions were presented by Cleland and Wilhelm (*2*), Lauwerier (*4*), and Wissler and Schechter (*9*). Wissler and Schechter used an eigenvalue solution and reported numerical results in agreement with the finite difference calculations of Cleland and Wilhelm. Chambre (*1*) has used a perturbation method and extended the problem to include finite heats of reaction. Studies of heterogeneous reactions in flow systems have been discussed briefly elsewhere (*8*), and additional details regarding parts of this paper are given in this reference also.

The simplest, and therefore most widely employed, geometries for the study of transport processes are circular tubes and infinite parallel plates. Superficially, hydrodynamic effects in these geometries seem similar, but obvious differences between them arise in some cases because of their two and three dimensional nature. For example, buoyancy effects in full-developed forced horizontal flows are quite different, since circulation occurs in tubes but not in the two dimensional system (*3*). Also it is often more convenient to study parallel plate systems experimentally. Therefore, since previous studies relate to homogeneous reaction in tube flows*, the case involving simultaneous homogeneous and heterogeneous reversible reaction in fully-developed isothermal laminar flow between parallel plates is considered here. These solutions also should approximate those for annuli under appropriate conditions.

SOLUTION OF THE STEADY STATE PROBLEM WITH NEGLIGIBLE AXIAL DIFFUSION

Consider a system in which reactant A undergoes a first-order reversible reaction, $A \rightleftharpoons B$, and enters an infinite parallel plate reactor with catalytic walls with a fully developed laminar velocity profile and a uniform concentration c_o. A mass balance for reactant A yields the following well-known differential equation:

$$u_m \left[1 - \left(\frac{y}{d} \right)^2 \right] \frac{\partial C}{\partial x} = D \left[\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right] - k_1 C + k_1' C_B \quad (1)$$

In dimensionless form Equations (1) and (2) become

$$(1 - \epsilon^2) \frac{\partial \theta}{\partial \beta} = \frac{\partial^2 \theta}{\partial \epsilon^2} + \frac{1}{N_{Pe}^2} \frac{\partial^2 \theta}{\partial \beta^2} - \alpha_1^2 \theta \quad (3)$$

and

$$\theta(0,\epsilon) = 1; \frac{\partial \theta(\beta,0)}{\partial \epsilon} = 0; - \frac{\partial \theta(\beta,1)}{\partial \epsilon} = \alpha_2^2 \theta(\beta,1) \quad (4)$$

The solution of Equation (3) for negligible axial diffusion can be obtained as usual in the form

$$\theta = \sum_{n=1}^{\infty} A_n e^{-\lambda_n \beta} Y_n(\epsilon) \quad (5)$$

in which the λ_n and $Y_n(\epsilon)$ are the eigenvalues and the eigenfunctions of the Sturm-Liouville system

$$\frac{d^2 Y_n}{d\epsilon^2} + [\lambda_n (1 - \epsilon^2) - \alpha_1^2] Y_n = 0 \quad (6)$$

with the conditions

$$\frac{d Y_n(0)}{d\epsilon} = 0; \frac{d Y_n(1)}{d\epsilon} = - \alpha_2^2 Y_n(1) \quad (7)$$

Then the A_n's are evaluated with the boundary condition at $\beta = 0$. Thus

$$A_n = - \frac{\left[\frac{\alpha_2^2}{\lambda_n} Y_n(1) + \frac{\alpha_1^2}{\lambda_n} \int_o^1 Y_n(\epsilon) d\epsilon \right]}{Y_n(1) \left[\alpha_2^2 \frac{d Y_n(1)}{d \lambda_n} + \frac{d}{d \lambda_n} \left(\frac{d Y_n(1)}{d\epsilon} \right) \right]} \quad (8)$$

The associated boundary conditions are

$$C(0,y) = C_o; \frac{\partial C(x,0)}{\partial y} = 0;$$

$$- D \frac{\partial C(x,d)}{\partial y} = k_2 C - k_2' C_B \quad (2)$$

The average concentration is defined as

$$\theta_{avg} = \frac{3}{2} \int_o^1 (1 - \epsilon^2) \theta \, d\epsilon \quad (9)$$

Equation (5) can be substituted into Equations (9) and (6) used to obtain

$$\theta_{avg} = \frac{3}{2} \sum_{n=1}^{\infty} A_n e^{-\lambda_n \beta} N_n \quad (10)$$

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* After the revision of this paper was completed, an article by J. S. Dranoff, *Chem. Eng. Sci.*, **17**, 706 (1962) appeared, and indicated calculations for tube flows with catalytic walls have been reported.

where N_n's are defined as

$$N_n = \frac{\alpha_2^2}{\lambda_n} Y_n(1) + \frac{\alpha_1^2}{\lambda_n} \int_0^1 Y_n(\epsilon)\, d\epsilon \tag{11}$$

For noncatalytic walls, the values of λ_n, $Y_n(\epsilon)$, A_n, and N_n can be found from Equations (6), (7), (8), and (1) by letting $\alpha_2 = 0$. The first four eigenvalues and the related constants A_n $Y_n(1)$ and N_n are tabulated elsewhere.* The average concentration distributions as a function of β with α_1 as parameter and $\alpha_2 = 0$ are presented in Figure 1. Comparisons with solutions obtained neglecting molecular diffusion and for plug flow are also shown in Figure 1. The effect of heterogeneous reaction at the wall is shown in Figure 2 for several values of α_1 and α_2.

For the irreversible reaction $A \rightarrow B$, the above solutions can be used by noting that K is infinite in this case. Thus θ and θ_{avg} are equivalent to C/C_o and $(C/C_o)_{avg}$.

AXIAL DIFFUSION EFFECTS

The effect of molecular diffusion in the direction of flow in heat transfer systems has been the subject of several theoretical studies (5, 6, 7). It is of interest to determine the magnitude of this effect when chemical reactions occur. Since the exact treatment requires rather extensive numerical work, it is logical to obtain first an estimate of the magnitude of this effect to determine whether or not an exact analysis is warranted. The well-known integral method is used for this purpose.

If one substitutes

$$\theta = \sum_{n=1}^{\infty} A_n X_n(\beta)\, Y_n(\epsilon)$$

into Equation (3) and integrates with respect to ϵ from 0 to 1, the following results:

$$\frac{d^2X_n}{d\beta^2} - \frac{N_{Pe}^2}{\lambda_n}\left[\alpha_1^2 + \frac{\alpha_2^2 Y_n(1)}{\int_0^1 Y_n\, d\epsilon}\right]$$
$$\frac{dX_n}{d\beta} - N_{Pe}^2\left[\alpha_1^2 + \frac{\alpha_2^2 Y_n(1)}{\int_0^1 Y_n\, d\epsilon}\right] X_n = 0$$

Using $X_n\ (\infty) \rightarrow$ o and the binomial theorem one gets as an approximation

$$X_n = e^{-\left\{\lambda_n - \frac{\lambda_n^3 \int_0^1 Y_n d\epsilon}{N_{Pe}^2\left[\alpha_1^2 \int_0^1 Y_n d\epsilon \,-\, Y_n'(1)\right]}\right\}\beta}$$

When one compares the coefficient of β in the exponential function with λ_n, this calculation indicates that the axial diffusion effect is negligible for $N_{Pe} \geqq 100$ even with rapid reactions. This corresponds with exact results obtained in heat transfer systems. In the very

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* Tabular material has been deposited as document 7426 with the American Documentation Institute, Photoduplication Service, Library of Congress, Washington 25, D. C., and may be obtained for $1.25 for photoprints or for 35-mm. microfilm.

INFORMATION RETRIEVAL*

Key Words: Unsteady State-1, Step Input-1, Rectangular Pulse Input-1, Sinusoidal Input-1, Frequency Response-2, Time Constant-2, Liquid-5, Phases-5, Velocity Fluid-6, Bed Height-7, Bed Porosity-7, Dynamics-8, Fluidization-8, Linear Model-10, Experimental-10.

Abstract: The dynamic response of bed height in liquid-solid fluidized beds to a change in fluidizing velocity was considered. A linearized model was developed such that the time constant for the system could be estimated with the parameters characterizing the system. The experimental response to step, rectangular pulse, and sinusoidal inputs in fluidizing velocity were measured.

Reference: Fan, Liang-Tseng, James A. Schmitz, and Eugene N. Miller, **A.I.Ch.E. Journal, 9,** No. 2, p. 149 (1963).

Key Words: A. Fluctuations-7, Mass Transfer-7, Rate-7, Diffusion-10, Electrode-10, Reaction-10, Reduction-10, Potassium Ferricyanide-5. B. Turbulence-8, Viscous Sublayer-8, Pipe-8, Wall-8. C. Average-9, Root-Mean-Square-9, Intensity-9, Correlation Coefficient-9, Integral Scale-9, Spectra-9. D. Elongated-, Flow Disturbances-8, Time Scale-8, Pipe Diameter-6, Average Velocity-6.

Abstract: Measurements of fluctuations in the mass transfer rate of the diffusion controlled electrode reaction, reduction of potassium ferricyanide, on a small circular electrode mounted flush with a pipe wall are used to study the unsteady nature of the viscous sublayer. A relation between mass transfer fluctuations and velocity gradient fluctuations at the wall is derived. From the analysis of measurements of average and root-mean-square transfer rates, correlation coefficients, and frequency spectra, it is concluded that flow disturbances in the viscous sublayer have intensities of at least ten percent, are elongated in the direction of flow, and are characterized by a time scale equal to the pipe radius divided by the bulk average velocity.

Reference: Reiss, L. Philip, and Thomas J. Hanratty, **A.I.Ch.E. Journal, 9,** No. 2, p. 154 (1963).

Key Words: Mass Transfer-8, Ratios-8, Unsteady State-10, Penetration-10, Reaction-8, Factors-6, Ratios-7, Distribution-6, Concentration-9, Temperature-9, Liquid Phase-9, Interface-9, Theory-8, Mechanism-8, Predictions-9, Rates-8, Coefficients-8, Chemical Properties-6, Physical Properties-6, Mass Transfer-7, Rates-7, Coefficients-7, Comparison-8, Diffusion-8, Diffusion-7, Heat Transfer-8, Diffusion-9, Hydrodynamics-6.

Abstract: Based on the film-penetration concept, a mathematical model to describe the mechanism of mass transfer accompanied by a first-order irreversible chemical reaction at the interface has been formulated. The film-penetration concept provides information which cannot be obtained by either the film theory or the surface renewal theory alone.

All the three theories predict practically the same effect of chemical reaction on the mass transfer rate, provided an accurate physical mass transfer coefficient is available. If not available, then, the choice of the theory to predict the chemical mass transfer rate may become critical.

Reference: Huang, Chen-Jung, and Chiang-Hai Kuo, **A.I.Ch.E. Journal, 9,** No. 2, p. 161 (1963).

Key Words: Hydrogen Peroxide-1, Reactor (Tubular)-10, Stainless Steel-4, Glass-4, Porous Wall-10, Diffusion-6, Catalysts-4, Inert Gas-5, Injection-6, Reaction Rate-7.

Abstract: This study explored some of the reaction characteristics of a novel type of reactor, consisting of a tube with a porous wall through which an inert gas could be passed to reduce diffusion of other species to the vessel surface. Studies were made with and without injection of inert gas through the porous wall with the heterogeneous decomposition of hydrogen peroxide vapor in the main stream as the model reaction.

Results without injection agree reasonably well with theory. Discrepancies between results of reaction with injection and theory are discussed. Concentration profiles along the reactor with wall injection but without reaction are given.

Reference: Satterfield, Charles N., Robert C. Reid, and Alfred E. Wechsler, **A.I.Ch.E. Journal, 9,** No. 2, p. 168 (1963).

(Continued on page 276)

* For details on the use of these key words and the A.I.Ch.E. Information Retrieval Program, see **Chem. Eng. Progr., 57,** No. 5, p. 55 (May, 1961), No. 6, p. 73 (June, 1961); **58,** No. 7, p. 9 (July, 1962).

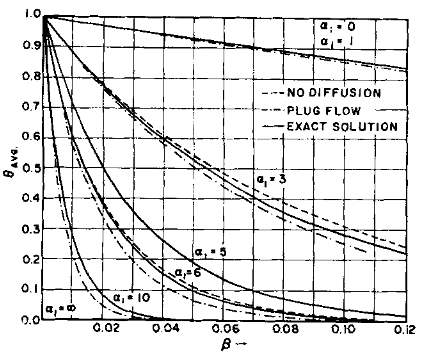

Fig. 1. Average concentration as a function of the distance for various values of α_1 with $\alpha_2 = 0$.

slow flow region $N_{Pe} < 100$ buoyancy effects due to density variations are pronounced, and the assumed velocity distribution is inapplicable. Thus it doesn't seem reasonable to study this effect rigorously unless bouyancy is also considered.

MASS TRANSFER WITH HOMOGENEOUS FIRST ORDER REACTION

The purpose of this section is to use the eigenfunction solutions obtained previously to determine the effect of chemical reaction in the flow on mass transfer from a wall. Consider a fluid B entering, in fully-developed flow, a system of two infinite parallel plates made of component A. Assume A is sparingly soluble in B and that a reaction takes place between A and B in the fluid but the concentration of B does not change substantially throughout the system; hence the reaction rate may be considered first order in A. Then the diffusion equation from component A may be written in dimensionless form as

$$(1-\epsilon^2)\frac{\partial\theta_1}{\partial\beta} = \frac{\partial^2\theta_1}{\partial\epsilon^2} - \alpha_1^2\left[\theta_1 + 1 - \frac{C_o}{C_e}\left(\frac{1}{K+1}\right)\right] \qquad (12)$$

with the boundary conditions

$$\theta_1(0,\epsilon) = \frac{C_o}{C_e} - 1 \qquad (13a)$$

$$\theta_1(\beta,1) = 0 \qquad (13b)$$

$$\frac{\partial\theta_1(\beta,0)}{\partial\epsilon} = 0 \qquad (13c)$$

In order to use the solutions obtained previously, Equation (13b) may be replaced by

$$-\frac{1}{\alpha_2^2}\frac{\partial\theta_1(\beta,1)}{\partial\epsilon} = \theta_1(\beta,1) \qquad (14)$$

Clearly Equation (14) is exactly equivalent to Equation (13b) when $\alpha_2^2 \to \infty$. However it has been found that $\alpha_2^2 \geqq 100$ yielded results that were, for practical purposes, equal to those for $\alpha_2^2 = \infty$.

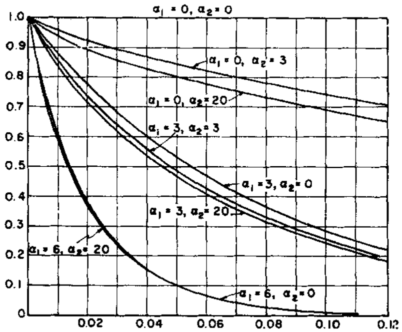

Fig. 2. Average concentration as a function of the distance for simultaneous homogeneous reaction in the flow and heterogeneous reaction at the wall.

Now let

$$\theta_1(\beta,\epsilon) = \theta_2(\epsilon) + \theta_3(\beta,\epsilon)$$

Thus $\theta_2(\epsilon)$ satisfies Equations (12), (13b), and (13c) and is easily found to be

$$\theta_2(\epsilon) = M\left\{\frac{\cosh\alpha_1\epsilon}{\cosh\alpha_1} - 1\right\}$$

where

$$M = 1 - \frac{C_o/C_e}{K+1}$$

Therefore $\theta_3(\beta,\epsilon)$ must satisfy

$$(1-\epsilon^2)\frac{\partial\theta_3}{\partial\beta} = \frac{\partial^2\theta_3}{\partial\epsilon^2} - \alpha_1^2\,\theta_3$$

together with

$$\theta_3(0,\epsilon) = \frac{C_o}{C_e} + M - 1 - M\frac{\cosh\alpha_1\epsilon}{\cosh\alpha_1} = L - M\frac{\cosh\alpha_1\epsilon}{\cosh\alpha_1} \qquad (15)$$

and Equations (13c) and (14). When the reaction is irreversible, $M = 1$ and $L = C_o/C_e$.

Assuming

$$\theta_3(\beta,\epsilon) = \sum_{n=1}^{\infty} B_n\,e^{-\lambda_n\beta}\,Y_n(\epsilon)$$

one obtains Equations (6) and (7) identically. Thus the Y_n and λ_n, to $n = 4$, have been calculated for α_2^2 up to 400 which, as previously stated, is essentially equal to $\alpha_2^2 = \infty$. This was verified for the present case by comparing the eigenvalues obtained for $\alpha_1^2 = 0$ with those obtained by Brown (1), and the agreement was quite good.

It remains to determine the B_n. Surprisingly, this turns out to be a remarkably simple matter. Using Equation (15) and the properties of the Sturm-Liouville system one gets

$$B_n = \frac{\displaystyle\int_0^1\left[L - M\frac{\cosh\alpha_1\epsilon}{\cosh\alpha_1}\right](1-\epsilon^2)Y_n\,d\epsilon}{\displaystyle\int_0^1(1-\epsilon^2)\,Y_n^2\,d\epsilon} \qquad (16)$$

The denominator of Equation (16) has already been calculated, and the numerator may be transformed by partial integration and some manipulation to yield

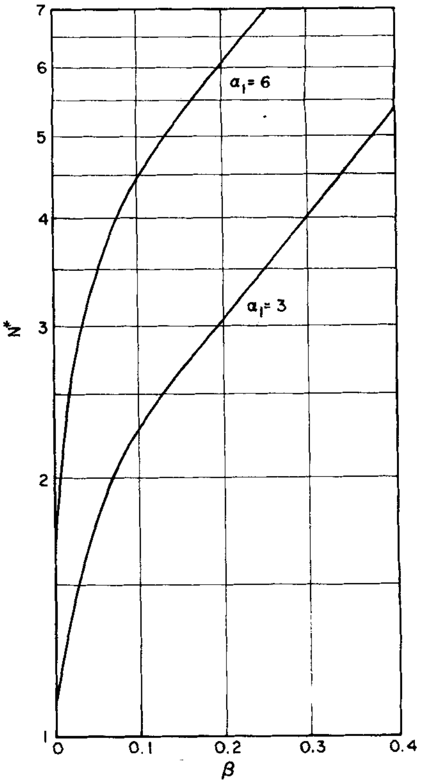

Fig. 3. Effect of chemical reaction of rate of mass transfer.

$$\int_0^1\left[L - M\frac{\cosh\alpha_1\epsilon}{\cosh\alpha_1}\right](1-\epsilon^2)Y_n\,d\epsilon = -\frac{1}{\lambda_n}\left[L\,(Y_n')(1) - \alpha_1^2\int_0^1 Y_n\,d\epsilon - M\,Y_n'(1)\right]$$

in which all of the terms have been computed previously.

A result of practical interest is the influence of chemical reaction on the rate of mass transfer. Figure 3 shows N^*, the ratio of the mass flux with irreversible reactions described by $\alpha_1 = 3$ and $\alpha_1 = 6$, to that without reaction. N^*_∞ is easily shown to be

$$N^*_\infty = 0.596\,\alpha_1\tanh\alpha_1\,e^{2.816\beta}$$

As expected from this asymptotic exponential form, N^* is linear in β on a semilog plot for sufficiently large β. For values of the reaction parameter considered here this asymptotic formula gives good results for $\beta \geqq 0.1$.

DISCUSSION OF RESULTS

Comparison of exact solutions with the limiting cases of no molecular diffusion and plug flow, which represents infinite radial diffusion, are presented in Figure 1. Solutions obtained by assuming negligible molecular diffusion approximate the exact solutions for large values of α_1. From the results one can conclude that for values of $\alpha_1 \geqq 10$ the average concentration can be obtained, with an error less than 2%, by neglecting molecular diffusion. This is

(*Continued from page 274*)

INFORMATION RETRIEVAL

Key Words: Mixing-8, Rates-8, Reactions-8, Heterogeneous-8, Dispersing-9, Immiscible-9, Liquid Phase-9, Contacts-9, Distributions-9, Residence-9, Mass Transfer-9, Segregation-9, Stirring-6, Mixing-6, Conversion-7, Selectivity-7, Statistics-10, Computers-10.

Abstract: A mathematical representation of dispersed phase mixing in a single-stage stirred reactor has been developed and used to compute the range of values for the mixing rate which lie between effectively mixed and unmixed conditions and the conversion occurring in this range. Examples are given for the effect of various mixing rates on the conversion and spread of concentration for non-first-order reactions or mass transfer rate controlled reactions in the dispersed phase.

Reference: Curl, R. L., **A.I.Ch.E. Journal, 9,** No. 2, p. 175 (1963).

Key Words: Benedict-Webb-Rubin-Friend Equation of State-8, Correlation-8, 2 Methyl *Paraffinic Hydrocarbons*-9, Compressibilities-2, 2 Methyl Propane-9, 2 Methyl Butane-9, 2 Methyl Pentane-9, Critical Pressures-2, 2 Methyl Hexane-9, 2 Methyl Heptane-9.

Abstract: The eight constants of the Benedict-Webb-Rubin-Friend equation of state have been correlated for the 2 methyl paraffinic hydrocarbons with critical temperature and structural properties as parameters.

Calculated compressibilities in the superheated vapor region with correlation constants deviated on the average by less than 1% for 2 methyl propane, 2 methyl butane, and 2 methyl pentane. Critical pressure values calculated similarly differed by 0.731 atm. (on the average) from experimental values.

Critical pressures for 2 methyl hexane and 2 methyl heptane calculated from extrapolated constants differed by 0.377 and 0.295 atm., respectively, from experimental values.

Reference: Griskey, Richard G., and Lawrence N. Canjar, **A.I.Ch.E. Journal, 9,** No. 2, p. 182 (1963).

Key Words: Natural Convection-7, Heat Transfer Coefficients-8, Hydrodynamic Stability-7, Turbulence-7, Heat Transfer-8, Unsteady Flow-7, Temperature Fluctuations-10, Pipe Heat Transfer-8, Low Reynolds Number Heat Transfer-8, Convective Heat Transfer-8.

Abstract: If water flowing through a vertical pipe is heated or cooled, natural convection effects can cause a transition to an unsteady flow. Measurements of the effect of this unsteady flow on the rate of heat transfer are presented for constant heat flux conditions. The marked differences noted between upflow and downflow experiments reflected the difference in the unsteady flows. Downflow transition led to a highly random flow field while upflow transition did not.

Reference: Scheele, George F., and Thomas J. Hanratty, **A.I.Ch.E. Journal, 9,** No. 2, p. 183 (1963).

Key Words: A. Optimization-8, Multidimensional-8, Elimination-10, Experimental Error-3, Economics-8, B. Global-8, Local-8, Response Surface-8, Contour-10, Tangent-10, Hyperplane-10, Unimodal-1, Strongly Unimodal-1. C. Elimination-10, Middle-10, Midpoint-10, Center of Volume-10, Centroid-10, Extrapolation-3. D. Gradient-10, Pilot Experiment-10, Climbing-8, Computer-10.

Abstract: Search problems involve finding the optimum of a function whose values can be determined only by direct experiment or computation. This article proposes a contour tangent search technique which by a process of elimination continually narrows down the region known to contain the optimum. The success of the technique depends on the function being strongly unimodal, a concept defined in the article. Experimental error rapidly reduces the effectiveness of the method, which, however, should find application in problems involving many independent variables.

Reference: Wilde, Douglass J., **A.I.Ch.E. Journal, 9,** No. 2, p. 186 (1963).

(*Continued on page 278*)

a tremendous simplification, since the eigenvalue problems become increasingly difficult from the practical view point for $\alpha_1 > 10$. The very simple plug flow solutions more closely approximate exact results for small values of α_1. With $\alpha_1 \leqq 1$, one may use the plug flow solution with an error less than 3% throughout the length of the reactor.

The eigenvalues determined for systems with catalytic walls tend asymptotically to a given value beyond $\alpha_2 = 10$ for every value of α_1. This means that increasing the value of α_2 from 10 up to infinity will not change the solution at all. Clearly, this is the case of a diffusion controlled reaction, where the possible rate of surface reaction is much faster than the rate of diffusion to the surface. Hence, the concentration at the surface is always its equilibrium composition. Clearly this property was useful in considering the case with mass transfer.

The faster the reaction in the flow, the smaller the effect of the catalyst. For $\alpha_1 = 6$ differences between average concentration profiles for $\alpha_2 = 0$ and $\alpha_2 = 20$ (or $\alpha_2 = \infty$) are quite small. However the point concentration at the wall with $\alpha_2 = 0$ is much higher than that for $\alpha_2 = \infty$. Hence one has different types of profiles with about the same average concentration. This can be explained by considering that the concentration distribution is different only for the region near the wall, while the contribution of this region to the bulk mean value is very small, since the velocity of the fluid approaches zero near the wall.

It is clear that axial molecular diffusion effects are important only at low values of N_{Pe}, even when the reaction rate is rather high. A relatively large value of the reaction parameter tends to increase the importance of axial diffusion by creating a steeper axial gradient. For $\alpha_1 = 8$, to obtain 95% conversion at $N_{Pe} = 30$ axial diffusion increases the required reactor length by about 6%, whereas at $N_{Pe} = 100$ the increase is negligible.

ACKNOWLEDGMENT

This research was sponsored in part by the Office of Saline Water.

NOTATION

A_n = expansion coefficients
C = concentration of component A
C_e = equilibrium concentration of component A at the wall
C_o = concentration of component A at entrance to system
D = diffusivity of component A
d = half distance between parallel plates

K = thermodynamic equilibrium constant
k_1 = reaction velocity constant in flow
k_2 = reaction velocity constant on catalyst surface
L = $\frac{C_o}{C_e} + M - 1$
M = $1 - \frac{C_o}{C_o}\left(\frac{1}{K+1}\right)$
N_{Re} = Reynolds number, $d\,Um\,\rho/\mu$
N_{Pe} = Peclet number, $N_{Re} \times N_{Sc}$
N_{Sc} = Schmidt number, $\mu/\rho D$
N^*_∞ = ratio of mass transfer rate with irreversible reaction to that without reaction at $\beta = \infty$
U_m = maximum velocity at $\epsilon = 0$
x = axial distance from entrance
y = radial distance from center of channel
Y_n = eigenfunctions

Greek Letters

α_1 = homogeneous reaction parameter, $\sqrt{\frac{k_1 d^2}{D}\left(\frac{K+1}{K}\right)}$
α_2 = heterogeneous reaction parameter, $\sqrt{\frac{k_2 d}{D}\left(\frac{K+1}{K}\right)}$
β = dimensionless axial distance, $x/N_{Pe}d$
ϵ = dimensionless radial distance, y/d
θ = dimensionless concentration function, $\frac{(K+1)(C/C_o)-1}{K}$
θ_1 = dimensionless concentration function, $\frac{C}{C_e} - 1$
λ_n = eigenvalues
μ = viscosity
ρ = density

LITERATURE CITED

1. Chambre, P., *Appl. Sci. Res.*, **9**, 157 (1960).
2. Cleland, F. A., and R. A. Wilhelm, *A.I.Ch.E. Journal*, **2**, No. 4, p. 489 (1956).
3. Gill, W. N., and Eduardo Del Casal, *ibid.*, **8**, 513 and 570 (1962).
4. Lauwerier, H. A., *Appl. Sci. Res.*, **A8**, 336 (1959).
5. Millsaps, K., and K. Polhausen, *Math. Rev.*, **18**, 538 (1957).
6. Schneider, P. J., Heat Transfer and Fluid Mechanics Institute (1956).
7. Singh, S. N., *Appl. Sci. Res.*, **7**, No. 5, p. 325 (1958).
8. Suwandi, M. S., Master's thesis, Syracuse University, Syracuse, New York (September, 1961).
9. Wissler, E. H., and R. S. Schechter, *Appl. Sci. Res.*, **A9**, No. 5, p. 334 (1960); **10**, No. 3, p. 198 (1961).

Dual Variational Statements Viewed from Function Space

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In a recent note (*2*) W. E. Stewart exploited certain dual variational principles, developed by Hill and Johnson to obtain bounds for the volumetric flow rate Q of an incompressible, homogeneous, Newtonian fluid in steady, rectilinear motion. More general methods are available however for obtaining bounds in linear problems; these methods are developed in functional analysis (*3*, *4*). The purpose of this communication is to point out the correspondence which exists between dual variational statements and geometric constructions in a function space and to suggest the power of the more general approach.

BASIC EQUATIONS

The mathematical representation of an incompressible, rectilinear motion in a conduit is

$$\nabla^2 w = -\frac{\mathcal{P}}{\mu}; \quad \frac{\partial w}{\partial z} = 0; \quad \text{in } S_o \qquad (1)$$
$$w = 0 \quad \text{on walls of duct}$$

Green's identity combined with Equation (1) yields

$$Q \equiv \int_{S_o} w\, dA = \frac{1}{\mathcal{P}} \int_{S_o} \mu \nabla w \cdot \nabla w\, dA = \frac{1}{\mathcal{P}} D(w, w) \qquad (2)$$

In order to obtain bounds for the volumetric flow rate Q it is necessary to obtain bounds for the rate of viscous dissipation per unit length of duct $D(w, w)$.

PROBLEM IN FUNCTION SPACE

The natural setting of a variational problem is a space (or set) composed of functions which represent conceivable dynamic states (velocity fields in the present example). Such a space of functions is infinitely dimensional, yet can be pictured in the same manner as the space of free vectors in three-dimensional analytic geometry by imagining a function as a vector. In this spirit the scalar product of two functions u and v in the space is defined to be

$$D(v, u) \equiv \int_{S_o} \mu \nabla v \cdot \nabla u\, dA \quad \mu > 0 \qquad (3)$$

The positive square root of the quadratic form $D(v, v) \geqslant 0$ constitutes a distance measure in units of viscous dissipation, in function space; consequently the dynamic states in the space can be partially ordered by assigning them specific units of dissipation. The most important item in function space analysis is Schwarz's inequality, which in the present case takes the form

$$D^2(v, w) \leqq D(v, v)\, D(w, w) \qquad (4)$$

If $D(u, v) = 0$, u and v are said to be orthogonal, $u \perp v$. With these tools available, Equation (1) can be recast in a function space setting.

Let v be a space of continuous functions (in x and y) which possess continuous derivatives inclusive of the second order and let N represent the set of all those functions in v which vanish on the walls of the duct; that is

$$N = [v : v = 0 \text{ on the walls of the duct}] \qquad (5)$$

Now all those functions in v which are orthogonal to every function in N are sorted out and placed in a set $N\perp$. To do this requires finding all $u \epsilon v$ (where ϵ means 'contained in') and $v \epsilon N$ such that

$$D(v, u) = 0$$

Every $v \epsilon N$ vanishes on L_o (the periphery of the duct), and consequently by the definition of $D(v, u)$ it is required that

$$\nabla^2 u = 0 \quad \text{in } S_o \qquad (6)$$

for all $u \epsilon N\perp$; that is

$$N\perp = [u : \nabla^2 u = 0 \text{ in } S_o]$$

Thus Equation (1) recast in a function space setting becomes

$$w \epsilon N \quad w - w_o \epsilon N\perp \qquad (7)$$

where w_o is any function satisfying

$$\nabla^2 w_o = -\frac{\mathcal{P}}{\mu} \quad \text{in } S_o \qquad (7a)$$

This formulation is represented geometrically in Figure 1, where any line perpendicular to N represents $N\perp + w_i$ and α is an arbitrary constant. From the orthogonality of N and $N\perp$ it follows that

$$D(w - w_1, w) = 0 \quad w_1 - w_o \epsilon N\perp \qquad (8)$$

Inequality (6) yields the desired upper bound for $D(w, w)$:

$$D(w, w) \leqq D(w_1, w_1) \qquad (9)$$

Therefore any function satisfying the differential equation but not the boundary conditions of (1) yields an upper bound when used in calculating the viscous dissipation of the system. The