taken into consideration, in contrast with Hoelscher's Figure 2. In fact, if n also varies, the shape of the velocity profile varies and consequently, if the volumetric flow rate is constant, B also varies.

Therefore, K_1 and K_2 are not only functions of the volumetric flow rate and of the kinetic constants, but also depend upon n. Thus it is not advisable to use them to make a comparison when variations of n occur.

Equations (4), (5), and (6), and Figure 2, as well as the notation, are quoted from Hoelscher's work.

NOTATION

A = reagent
B see the equation of the velocity profile $V = B(1 - \sigma^n)$, cm./s
C = concentration, moles/cc.
k_1 = rate constant of step 1, s^{-1}
k_2 = rate constant of step 2, s^{-1}
K_1 = $k_1 \frac{L}{B}$, adim
K_2 = $k_2 \frac{L}{B}$, adim
L = reactor length, cm.
n = constant in the equation of the velocity profile $V = B\ (1 - \sigma^n)$, adim
r = radial distance measured from axis of tube, cm.
R = intermediate product
$\overline{R}$ = radius of the tube, cm.
t = reaction time, s
Y = $\dfrac{C_R}{C_{Ao}\left(\dfrac{k_1}{k_2 - k_1}\right)} = e^{-k_1 t} - e^{-k_2 t}$ modified concentration ratio, adim
V = local velocity, cm./s
σ = dimensionless position variable = $\frac{r}{\overline{R}}$, adim

Subscripts

m = mean value
o = initial value
pf = plug flow value
c = particular radial position $\leqq 1$

On the Minimum Time Operation of a Batch Reactor

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In a recent paper Cotter (*1*) treats the control problem of the minimum time operation of a batch reactor with a single exothermic reaction controlled by a cooling coil. The control variable is a function of the cooling water rate, and it is proved that the optimal control is bang-bang. The main purpose of this present paper is to establish that for the time-optimal problem considered by Cotter the optimal control is bang-bang with, at most, one discontinuity point. Furthermore, the same result is established for various systems more general than the system considered by Cotter (*1*). The control theory terminology of Pontryagin et al. (*2*) is used throughout the paper. An assumption for the analysis is that an optimal control exists for the time-optimal problems under consideration. Some aspects of the present paper have also been discussed from a more general point of view by Hermes and Haynes (*3*).

MINIMUM TIME OPERATION OF A BATCH REACTOR

Cotter (*1*) treats the problem of the minimum time operation of a batch reactor with a single exothermic reaction controlled by a cooling coil. The reaction is pseudo first order. Cotter considers an irreversible reaction with

$$\text{rate} = -xk_1(T) \qquad (1)$$

The system equations are given by

$$\frac{dx}{dt} = \frac{-xVk_1(T)}{W_x} \qquad (2)$$

$$\frac{dT}{dt} = \frac{VH_r k_1(T)}{W_T} - \frac{(T - T_o)\,\varphi}{W_T} \qquad (3)$$

For Equations (2) and (3) Cotter chooses the function φ as the control variable and assumes the state variables are given initially by $x(t_o)$, $T(t_o)$ and at the final time by $x(t_1)$, $T(t_1)$. In the terminology of Pontryagin (*2*), the time-optimal problem consists of determining an admissible control $\varphi(t)$ that transfers the phase point $x(t_o)$, $T(t_o)$ to the phase point $x(t_1)$, $T(t_1)$ in least time. In reference *1*, admissible controls are piecewise continuous functions in $t_o \leqq t \leqq t_1$. Cotter establishes that the optimal control is bang-bang (*1*).

PROBLEM FORMULATION

We shall analyze the problem treated by Cotter by considering a more general system of first-order differential equations.

$$\frac{dz_1}{dt} = A_1(z_1, z_2) \qquad (4)$$

$$\frac{dz_2}{dt} = B_1(z_1, z_2) + B_2(z_1, z_2)y \qquad (5)$$

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A pitot tube method for measuring the first normal stress difference and its influence on laminar velocity profile determinations, Savins, J. G., **A.I.Ch.E. Journal, 11,** No. 4, p. 673 (July, 1965).

Key Words: A. Measurement-8, Stresses-9, 6, Pitot Tube-10, Determination-7, Velocity Profile-9, Laminar Flow-9, Poiseuille Flow-9, Viscoelastic Fluids-9. B. Viscoelastic Fluids-9, Thickness-8, Boundary Layer-9, Nonlaminar Flow-9.

Abstract: A scheme is outlined that enables the calculation of the normal stress difference P_{11}-P_{22} in fluids undergoing steady Poiseuille flow from measurements with a pitot tube of local velocity distributions. This new technique should enable measurements in a region of shear rate comparable to that encountered in the torsional and circular flow methods. The presence of finite normal stresses should produce significant aberrations on the measurement of the velocity profile in the laminar flow of viscoelastic fluids. The presence of a P_{11}-P_{22} induced aberration on the velocity profile measurement suggests that caution be exercised in the practice of deducing estimates of the thickness of a boundary layer in the nonlaminar flow of these fluids.

Determination of plate efficiencies from operational data: Part II, Davis, Parke, D. L. Taylor, and C. D. Holland, **A.I.Ch.E. Journal, 11,** No. 4, p. 678 (July, 1965).

Key Words: A. Determination-8, Efficiency-9, 8, Plate Efficiency-9, 8, Distillation-9, 8, Distillation Columns-9, 8, Operational Data-10, Composition-10, Vapor-9, Liquid-9, Enthalpy-10, Boiling Point-10, Flow Rate-10, Subunits-10, Temperature-10, Distributions-10, Products-9, Computer-10.

Abstract: This paper has two primary objectives: (1) the extension of previous methods for the determination of plate efficiencies from column performance data, and (2) the interpretation and presentation of the efficiencies determined for a variety of commercial columns. The previous methods used any number of plate temperatures and any number of product distributions to determine a set of plate efficiencies. These methods were restricted to conventional columns.

The method described herein extends these basic methods to make use of any liquid or vapor compositions which may be known. In addition, the method is applicable to complex columns for which the compositions, flow rates, and thermal conditions of each sidestream are known. The method involves the resolution of such columns into two or more simple, independent units that are referred to as subunits.

Axial dispersion during pulsating pipe flow, Taylor, Harry M., and Edward F. Leonard, **A.I.Ch.E. Journal, 11,** No. 4, p. 686 (July, 1965).

Key Words: A. Pulsations-8, 6, Dispersion-7, 8, Mixing-7, 8, Axial-0, Turbulent-0, Fluids-9, Flow-9, Unsteady-0, Periodic-0, Pipes-9, Round-0, Experimental-0, Frequency Response-10, Analog Computer-10, Digital Computer-10.

Abstract: A method is developed for the treatment of data obtained from flow systems whose performance is unsteady and periodic. Experimental results from a study of axial dispersion in pulsating turbulent flow in an open, round pipe are presented; they show that pulsations can greatly increase axial mixing.

Heat transfer in a round tube with sinusoidal wall heat flux distribution, Hsu, Chia-Jung, **A.I.Ch.E. Journal, 11,** No. 4, p. 690 (July, 1965).

Key Words: A. Heat Transfer-8, Tube-9, Round Tube-9, Sinusoidal-0, Heat Flux-8, Laminar Flow-9, Eigenvalues-8, 9, Eigenfunctions-8, 9, Nusselt Numbers-8, Asymptotic Expressions-8, Slug Flow-9, Mass Transfer-8, Mass Flux-8.

Abstract: *Sufficiently accurate values of first twenty eigenvalues, eigenfunctions,* and the coefficients for series expansion, as well as asymptotic expressions for these quantities, have been obtained for heat (or mass) transfer to fully developed laminar flow inside a round tube with uniform wall heat (or mass) flux. The first ten eigenfunctions are shown graphically for the radius range $0 \leq r/r_0 \leq 1$. These quantities are used to calculate the Nusselt numbers for sinusoidal wall heat flux distribution and compared with the corresponding slug flow Nusselt numbers.

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where the vector space Z of the vector variable $Z = (z_1, z_2)$ is the phase space of the object under consideration. In order to be able to use the maximum principle developed in reference 2 we shall require

$$A_1, B_1, B_2 \text{ to be continuous in } z_1, z_2 \tag{6}$$

and, in addition

$$A_1, B_1, B_2 \text{ to be continuously differentiable with respect to } z_1, z_2 \tag{7}$$

The control region is given by the closed set

$$Y : y_1 \leq y \leq y_2. \tag{8}$$

An admissible control is defined as an arbitrary piecewise continuous control with range in Y. As in reference 2, we define the time-optimal problem as follows.

In the phase space Z, two points, $z(t_0)$ and $z(t_1)$ are given. Find the admissible control (if such a control exists) that transfers the phase point $z(t_0)$ to the phase point $z(t_1)$ in least time.

MAXIMUM PRINCIPLE

We first construct the Hamiltonian as defined in reference 2, for Equations (4) and (5)

$$H = \psi_1 A_1 + \psi_2(B_1 + B_2 y), \tag{9}$$

where ψ_1, ψ_2 are the adjoint variables satisfying

$$\frac{d\psi_1}{dt} = \frac{-\partial H}{\partial z_1} = -\psi_1 \frac{\partial A_1}{\partial z_1} - \psi_2 \left(\frac{\partial B_1}{\partial z_1} + \frac{\partial B_2}{\partial z_1} y \right) \tag{10}$$

$$\frac{d\psi_2}{dt} = \frac{-\partial H}{\partial z_2} = -\psi_1 \frac{\partial A_1}{\partial z_2} - \psi_2 \left(\frac{\partial B_1}{\partial z_2} + \frac{\partial B_2}{\partial z_2} y \right) \tag{11}$$

Using a theorem on time-optimality established in reference 2,* we state that for $z(t)$ and $y(t)$ to be time-optimal it is necessary that there exists a nonzero continuous vector function $\psi(t) = \psi_1(t), \psi_2(t)$ corresponding to $y(t)$ and $z(t)$ such that

1° for all t, $t_0 \leq t \leq t_1$ the function $H(\psi, z, y)$ of the variable $y \epsilon Y$ attains its maximum at the point $y = y(t)$

$$H(\psi(t), z(t), y(t)) = M(\psi(t), z(t)) \tag{12}$$

* Theorem 2, p. 20.

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2° for all t, $t_0 \leqq t \leqq t_1$

$$M(\psi(t), z(t)) \geqq 0 \qquad (13)$$

For 2° to hold we require that $\psi(t)$, $z(t)$ and $y(t)$ satisfy both Equations (4) and (5) as well as Equations (10) and (11).

OPTIMAL CONTROLS

In this section we shall make use of the 1° and 2° of the maximum principle given in Equations (12) and (13). First, we shall make the following assumptions for the functions A_1, B_2 appearing in Equations (4) and (5).

$$A_1(z_1, z_2) < 0, B_2(z_1, z_2) < 0, \quad \frac{\partial A_1}{\partial z_2} < 0, \quad \text{all } z_1, z_2 \qquad (14)$$

From 1° of the maximum principle, as given in (12), the Hamiltonian is maximized with respect to the control variable y. From (8), (9), and (14) we can classify the control according to the value of ψ_2 on some nonzero time interval, as follows:

$$\psi_2 > 0, y \equiv y_1 \qquad (15)$$

$$\psi_2 \equiv 0, y_1 \leqq y \leqq y_2 \qquad (16)$$

$$\psi_2 < 0, y \equiv y_2 \qquad (17)$$

The function ψ_2 is commonly referred to in the literature as a *switching function.* Since the adjoint vector $\psi(t) = (\psi_1, \psi_2)$ is nonzero, it follows that $\psi_1(t)$ does not vanish at any time for which (16) holds. It then follows from (11) and (14) that $\psi_2(t)$ cannot vanish identically on some nonzero time interval. We have then rejected the possibility given by (16) and conclude that either (15) or (17) can hold. We describe this result by saying the optimal control is bang-bang.† First we define a switching point by a time t^* at which the control is discontinuous. From (15) and (17)

$$\psi_2(t^*) = 0 \qquad (18)$$

Following the convention used in reference 2 we choose

$$y(t^*) = y(t^* - 0). \qquad (19)$$

This convention indicates that at the switching point the control is given by its left-hand limit. From (9), (13),

† This bang-bang property of the optimal control can be established from reference 3 for systems more general than (4) and (5). If the functions Δ, ω (defined in reference 3) do not vanish for all x_1, x_2 then it follows that the optimal control is bang-bang. The purpose of this paper is to prove that the optimal control is bang-bang for (4) and (5) with, at most, one discontinuity point.

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Optimum design of conventional and complex distillation columns, Srygley, J. M., and C. D. Holland, **A.I.Ch.E. Journal, 11,** No. 4, p. 695 (July, 1965).

Key Words: A. Design-8, 9, 7, Distillation Columns-9, Columns (Process)-9, Optimization-8, Temperature-6, Separations-6, Purity-6, Number-7, 9, Distillation Trays-9, Theta Method of Convergence-10, Computer-10, Calculations-10.

Abstract: A method is proposed for achieving the optimum design, in the sense of minimum plates, for conventional and complex distillation columns for any set of specifications directly dependent on product purity that might be imposed by the designer. The method uses the calculational procedure of Thiele and Geddes, the θ method of convergence, and sequential-search procedures. Illustrative examples chosen from a large number of design problems solved by this method are presented.

The study of multicomponent gas-solid equilibrium at high pressures by gas chromatography: Part II. Generalization of the theory and application to the methane-propane-silica gel system, Gilmer, H. B., and Riki Kobayashi, **A.I.Ch.E. Journal, 11,** No. 4, p. 702 (July, 1965).

Key Words: A. Equilibrium-8, Gas-1, Solid-5, Methane-1, Propane-1, Silica Gel-5, High Pressure-5, Chromatography-10, Adsorption-2, Thermodynamics-7, Radioactive Tracers-10, Hydrocarbon-1. B. Apparatus-8, Radioactive Tracers-10.

Abstract: General relations to calculate the amount of each component of an elution gas adsorbed in a gas-solid system have been derived. This requires perturbations by radioactive tracers to obtain the retention volumes when multicomponent elution gases are used. Measurements were made at 20°C. up to 1,000 lb./sq.in.abs.

Diffusion in the laminar boundary layer with a variable density, Hanna, Owen T., **A.I.Ch.E. Journal, 11,** No. 4, p. 706 (July, 1965).

Key Words: Diffusion-8, 7, Isothermal-0, Mixture-9, Gases-9, Binary-0, Boundary Layor-9, Laminar-0, Density-6, Convection-8, 7, Forced-0, Free-0, Laminar Flow-9, Schmidt Number-6, Mass Transfer-6.

Abstract: The problem of isothermal diffusion in a variable molecular-weight binary gas mixture is considered for the case when the process occurs in a laminar boundary layer. Viscosity and diffusion coefficient are assumed constant. Solutions are given for both forced and free convection at large Schmidt numbers and large mass transfer rates toward the surface.

Interstage mixing in an Oldshue-Rushton liquid-liquid extraction column, Gutoff, Edgar B., **A.I.Ch.E. Journal, 11,** No. 4, p. 712 (July, 1965).

Key Words: A. Interstage Mixing-8, 7, Oldshue-Rushton Column-9, Liquid-Liquid Extraction-10, Agitated Columns-9, Brine-1, 2, Water-1, Velocity-6, Agitator-9, Backflows- 7, 8, Eddy Diffusivities-7, 8, Turbulence-6, Agitation-6, B. Design-8, Baffle Plates-9, Horizontal-0.

Abstract: Interstage mixing was measured in a 4-in. diam. Oldshue-Rushton column fed with a salt solution at the top and distilled water at the bottom, with the diluted salt solution leaving at the top. Mixing between stages is relatively slight at low agitator speeds, but increases very rapidly with speed once the turbulent region is reached. Interstage mixing is reported in terms of bulk backflows and also in terms of eddy diffusivities. The amount of interstage mixing is similar to that reported in the literature for rotating disk contactors. Variations in the horizontal baffle plate design were also studied.

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(14), and (18) we get that at a switching point t^*

$$\psi_1(t^*) < 0 \qquad (20)$$

We note the strict inequality in (20) since the adjoint vector cannot vanish at t^*. From (11), (14), (18), and (20) we get

$$\left.\frac{d\psi_2}{dt}\right|_{\substack{t=t^*\\ \psi_2=0}} < 0 \qquad (21)$$

It has been established that the optimal control is bang-bang. Let us assume the control on some nonzero time interval is at the upper limit y_2 given in (8) and a switching takes place at t^*. We have from (15) that for some nonzero time interval $t_a \leq t < t^*$.

$$\psi_2 < 0, y \equiv y_2, t_a \leq t \leq t^* \qquad (22)$$

It follows from (18) and (21) that there exists a positive δ so that

$$\psi_2 < 0, t^* < t < t^* + \delta \qquad (23)$$

We then get from (17) and (23)

$$y \equiv y_2, t^* < t < t^* + \delta \qquad (24)$$

However, (24) contradicts the assumption that the optimal control is switched at t^* from the upper level y_2. We can describe this result by saying that if the optimal control is at the upper level a switching cannot take place. If the optimal control is initially at y_2 it remains at y_2 for the entire process; that is from (15)

$$\psi_2|_o < 0, y \equiv y_2, \text{all } t \text{ in } t_o \leq t \leq t_1 \qquad (25)$$

The next possibility to consider is that the optimal control is initially at the lower level y_1 given in (8) and a switching takes place at t^*. With the control at the upper level y_2 it has been established that no switchings can take place. We describe this possibility as follows:

$$\psi_2 > 0, y = y_1, t_o \leq t \leq t^* \qquad (26)$$

$$\psi_2 < 0, y = y_2, t^* < t \leq t_1 \qquad (27)$$

We can sum up the results given in (25), (26), and (27) by the following theorem.

THEOREM

For Equations (4) and (5) under the assumptions (6), (7), (14) the time-optimal control is bang-bang with, at most, one switching point.

We briefly state without proof that this theorem can be strengthened by relaxing the requirement in (14) to read

$A_1(z_1, z_2) \neq 0, B_2(z_1, z_2) \neq 0,$

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$$\frac{\partial A_1}{\partial z_2} \neq 0, \text{ all } z_1, z_2 \quad (28)$$

We conclude this section by noting that the results of the theorem apply to Equations (2) and (3) considered by Cotter. We shall first require that the assumptions for the system corresponding to (6) and (7) are satisfied. We next observe that the requirement given in (14) is satisfied, since the functions

$$x > 0, k_1(T) > 0, \frac{dk_1}{dT} > 0, \quad (T - T_o) > 0 \quad (29)$$

and the parameters

$$V > 0, W_x > 0, W_T > 0, H_r > 0, \quad (30)$$

for the process. We conclude that the time-optimal control for (2) and (3) considered by Cotter has, at most, one switching point. This result extends the result of Cotter, who had previously established that the optimal control is bang-bang.

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NOTATION

H = Hamiltonian
H_r = heat of reaction
$k_1(T)$ = specific reaction velocity
T = reaction temperature
T_o = the cooling water temperature at coil inlet
V = reactor contents volume
W_T = molar heat capacitance of reactor contents
W_x = moles in reactor
x = reactant mole fraction
y = control variable
φ = nonlinear function of cooling water flow rate (control variable)
ψ_1 = adjoint variable
ψ_2 = adjoint variable (switching function)

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