COMMUNICATIONS TO THE EDITOR

An Example of the Use of Combined Models: Mixing in a Tubular Reactor with Return Bends

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Recently, some data on axial mixing in a tubular high-pressure reactor with a large proportion of return bends were presented by Carter and Bir (*4*). They found, as would be qualitatively expected, that the axial mixing was somewhat greater than that observed for straight pipe flow. Thus, they concluded that more experimenetal work is needed for systems of this type.

It would seem that a reactor of this type could be broken up naturally into two sections. First, the straight, tubular part, and second, the return bends. The axial mixing in the straight portion could be found then from correlations such as Levenspiel's (*6*), and the bends might be approximately treated as perfect mixers. This latter approximation is probably a rather poor one, since the bends would not act as perfect mixers under all flow conditions. A better representation could be found by experimentally measuring mixing in bends, but this information is not available at the present time. Thus the results of the analysis to be presented will be limited to relatively crude estimates of the total axial dispersion and will serve more as an indication of what could be done if more data were available.

Models of this type, which were given the name of *mixed models* or *combined models* (*9*), and organized and generalized by Levenspiel (*7*) have been found to be useful in other types of complex flow situations. Thus, one of the earlier applications was to the flow in fluidized beds as discussed, for example, by May (*10*). Another application to flow in real stirred tanks was by Cholette and Cloutier (*5*). The advantages of such a procedure are mainly that the mixing characteristics of each individual section may be obtained from standard correlations such as those for empty pipes, perfectly mixed regions, etc., and then combined for the total system. Thus, the very extensive experimental testing of every possible type of system made up of combinations of the single elements, which would be almost impossible, is avoided. The correlation of mixing data then becomes less voluminous.

DEVELOPMENT OF MODELS

The model that lumps the straight-pipe and return-bend mixing into one effective axial dispersion coefficient, as used by Carter and Bir, is represented

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Kihara and Lennard-Jones Parameters for the Isomeric Hexanes

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Precise methods of estimating physical data are quite useful and are often the sole source of such information for the process engineer. One such method is the estimation of transport properties (*1* to *4*) using the parameters of the Lennard-Jones intermolecular potential (*5*):

$$U(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \tag{1}$$

Another technique is the estimation of vapor-liquid equilibrium constants (*6*) using parameters of the Kihara intermolecular potential (*7*):

$$U_\rho = U_o\left[\left(\frac{\rho_o}{\rho}\right)^{12} - 2\left(\frac{\rho_o}{\rho}\right)^{6}\right] \tag{2}$$

The Lennard-Jones potential assumes a spherical molecule with *r*-to-*r* spacing between molecules. Although specifically designed to describe spherical molecules, it is applicable to nonspherical molecules, especially over short temperature ranges.

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TABLE 1. KIHARA AND LENNARD-JONES PARAMETERS FOR THE ISOMERIC HEXANES

Compound	l_1	l_2	l_3	V_o	S_o	M_o	ρ_o	U_o/k	σ(Å)	ϵ/k (°K.)
2,2-dimethylbutane	0.862	0.543	2.51	3.35	39.6	17.65	2.50	1060	7.614	266
2,3-dimethylbutane	0.783	0.788	1.57	4.02	30.8	19.65	2.50	1070	6.751	412
2-methylpentane	0.783	0.684	2.51	3.35	36.7	18.4	2.50	1130	8.065	267
3-methylpentane	0.862	0.543	2.51	3.35	35.3	17.6	2.50	1178	8.587	265

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The Relationship between the Froude and Reynolds Numbers in Falling Vertical Films

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Numerous workers in the field of falling liquid films have accepted the Froude number as a very appropriate dimensionless group for correlating their experimental results (*1, 2, 14*). Jackson (*14*) used the Froude number in the form

$$N_{Fr}' = \frac{V}{(gm)^{1/2}} \tag{1}$$

as a criterion for wave inception on films. His definition of the Froude number in this way must have been influenced by the fact that long gravity waves in a shallow, horizontal, open

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by the following differential equation:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D_e\frac{\partial^2 C}{\partial x^2} \qquad (1)$$

The boundary conditions correspond to those used by Carter and Bir:

$$C(x, 0) = 0 \qquad (2a)$$

$$\lim_{x\to\infty} C(x, t) = \text{finite} \qquad (2b)$$

$$C(0, t) = C_0(t) \qquad (2c)$$

The last boundary condition merely states that a tracer is to be injected at $x = 0$.

The combined model will next be formulated and is shown in Figure 1. For the i^{th} unit, the equations for the straight and the perfectly mixed or backmix portions are as follows:

$$\frac{\partial C_{pi}}{\partial t} + u\frac{\partial C_{pi}}{\partial x} = D\frac{\partial^2 C_{pi}}{\partial x^2} \qquad (3)$$

$$V_{bi}\frac{dC_{bi}}{dt} = v(C_{in,i} - C_{bi}) \qquad (4)$$

The boundary conditions are as follows:

$$C_{pi}(x, 0) = 0 \qquad (5a)$$

$$C_{pi}(0, t) = C_{bi} \qquad (5b)$$

$$\lim_{x\to\infty} C_{pi}(x, t) = \text{finite} \qquad (5c)$$

$$C_{bi}(0) = 0 \qquad (6a)$$

$$C_{in,i}(t) = C_{pi-1}(L_{pi}, t) \qquad (6b)$$

The value of D in Equation (3) is now the usual one for straight pipe flow as correlated by Levenspiel (*6*).

RELATING MODELS AND COMPARISON WITH EXPERIMENTAL DATA

In order to relate the model using the effective axial dispersion coefficient for the entire system to the combined model that considers the detailed parts of the system, the time moments of the tracer output curves are compared. This method was originally proposed for perfect impulse inputs by Levenspiel and Smith (*8*) and then generalized by Van der Laan (*11*). Aris (*2*) showed for axial dispersion that by using differences between the moments of the input and output, the restriction to perfect impulses could be removed. This was later generalized by Bischoff (*3*) to apply to any model. This paper

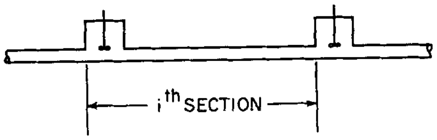

Fig. 1. Diagram of a combined model used to represent the reactor with return bends.

INFORMATION RETRIEVAL

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An experimental investigation of the inherent uncertainty in pool boiling critical heat fluxes to saturated water, Gambill, Wallace, **A.I.Ch.E. Journal, 10,** No. 4, p. 502 (July, 1964).

Key Words: Heat-1, Surface Deposit-3, Repetition-6, Liquid Level-6, Heat Transfer-7, Boiling-8, Vaporization-8, Superheat-8, Burnout-8, Water-9, Heating-10.

Abstract: A series of 234 critical-flux determinations conducted with atmospheric saturated water outside horizontal, resistance heated, nickel tubes protected from physical burnout revealed that under conditions of minimum surface variability there is an inherent uncertainty of $\sim \pm 9\%$ in the critical heat flux; the critical heat flux can vary significantly with the nature and condition of the surface; and even at very low liquid levels substantial heat fluxes ($\sim 10^5$ B.t.u./hr.sq.ft.) can be transferred without overheating of the tube wall.

Effects of reduced gravity on nucleate boiling bubble dynamics in saturated water, Siegel, R., and E. G. Keshock, **A.I.Ch.E. Journal, 10,** No. 4, p. 509 (July, 1964).

Key Words: Heat Transfer-9, Boiling-7, Nucleation-8, Bubbles-8, Water-5, Reduced Gravity-6, Evaporation-8, Heat-8, Fluxes-7, Motion-7, Size-7.

Abstract: Nucleate boiling bubble dynamics in distilled saturated water was studied in several reduced gravity fields ranging from 1.4 to 100% of earth gravity by placing the apparatus on a counterweighted falling platform. The nucleation occurred on a smooth horizontal surface at low heat fluxes. Only a few nucleation sites were active, so that nearly ideal individual bubbles were photographed. Measurements and comparisons with theory were made for bubble departure diameters and frequencies, growth rates, contact angles, base circle diameters, and rise velocities.

Turbulent disruption of flocs in small particle size suspensions, Thomas, David G., **A.I.Ch.E. Journal, 10,** No. 4, p. 517 (July, 1964).

Key Words: Flocculated Suspensions-1, Deflocculated Suspensions-2, Liquid-4, Water-4, Turbulent Energy Dissipation-6, Shear Rate-6, Yield Stress-6, Floc Size-7, Deflocculation-8, Flocculated Particles-9, Agglomerates-9, Turbulence-10, Laminar Shear-10.

Abstract: In the absence of turbulent fluctuations the main effect of a velocity gradient on the floc properties is a rearrangement of particles within the floc producing a more dense floc structure.

Under turbulent flow conditions the principle mechanism leading to floc rupture is pressure differences on opposite sides of the floc which cause bulgy deformation and rupture. The breakup of the floc is resisted by the yield stress τ_y and is promoted by an increase in the energy dissipation per unit mass of fluid ϵ.

Semibatch operation of a recirculation reactor for the hydrogenation of ethylene, Leinroth, J. P., Jr., and T. K. Sherwood, **A.I.Ch.E. Journal, 10,** No. 4, p. 524 (July, 1964).

Key Words: Ethylene-1, Hydrogen-1, Ethane-2, Catalyst-4, Copper-4, Reaction Rate-7, Hydrogenation-8, Kinetics-8, Reactions-8, Reactor-10, Recirculation Reactor-10, Semibatch Reactor-10, Batch, Circulation, Continuous, Flow, Recirculation-.

Abstract: This paper investigates semibatch operation of a recirculation reactor in kinetic studies wth ethylene hydrogenation over a supported copper catalyst being the specific reaction studied. In the semibatch method the reactor is operated continuously; then the outlet is abruptly shut off. Either hydrogen or ethylene is fed continuously to the reactor at a rate required to hold pressure constant. The reaction rate is directly equal to feed rate. Kinetics are studied at atmospheric pressure, 50° to 70°C., and at constant partial pressure of one of the reactants. Supplemental gas adsorption studies are made.

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is concerned only with the first two (dimensionless) moments, which could be found by solving Equations (1) through (6) as discussed in the above references.

Perhaps a simpler method of doing this is to utilize the fact that the mean and variance for a set of linearly connected independent distributions are additive. Thus the difference in (dimensionless) moments for each type of simple section can be taken from the literature (2, 3, 9).

Overall axial dispersion model:

$$\Delta\mu_1 = 1 \qquad (7a)$$

$$\Delta\sigma^2 = 2\frac{D_e}{uL} \qquad (7b)$$

All dispersion sections in combined model:

$$\Delta\mu_{1p} = \left(\frac{L_p}{L}\right) \qquad (8a)$$

$$\Delta\sigma_p{}^2 = 2\frac{D}{uL_p}\left(\frac{L_p}{L}\right)^2 \qquad (8b)$$

All backmix sections in combined model:

$$\Delta\mu_{1b} = \left(\frac{V_b}{V}\right) = \left(\frac{L_{b\,eq}}{L}\right) \qquad (9a)$$

$$\Delta\sigma_b{}^2 = \frac{1}{n}\left(\frac{V_b}{V}\right)^2 = \frac{1}{n}\left(\frac{L_{b\,eq}}{L}\right)^2 \qquad (9b)$$

The ratios of lengths in Equations (8) and (9) are used to put the moments on the same dimensionless basis. For the total combined model, Equations (8) and (9) when added give

$$\Delta\mu_1 = \frac{L_p}{L} + \frac{L_{b\,eq}}{L} = 1 \qquad (10a)$$

$$\Delta\sigma^2 = 2\frac{D}{uL}\frac{L_p}{L} + \frac{1}{n}\left(\frac{L_{b,\,eq}}{L}\right)^2 \qquad (10b)$$

The differences in (dimensionless) first moments for the two models, Equations (7*a*) and (10*a*), are consistent and state that the difference in means of the tracer curves is equal to the mean holding time. Equating the (dimensionless) variances for the two models gives the relationship sought between the models:

$$\frac{D_e}{uL} = \frac{D}{uL}\frac{L_p}{L} + \frac{1}{2n}\left(\frac{L_{b\,eq}}{L}\right)^2 \qquad (11)$$

Equation (11) can be modified to

$$\frac{D_e}{ud_t} = \frac{D}{ud_t}\left(\frac{L_p}{L}\right) + \frac{1}{2}\frac{L_i}{d_t}\left(\frac{L_{b\,eq}}{L}\right)^2 \qquad (12)$$

Each of the geometrical factors (L_p/L), $(L_{b\,eq}/L)$, and (L_i/d_t) are independent of the total number of sections in the system. This agrees with one of the experimental observations of Carter

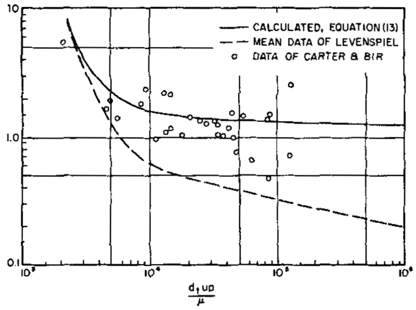

Fig. 2. Comparison of measured axial dispersion coefficients with those from the combined model.

and Bir that the effective dispersion coefficient was independent of the total length of test section.

In order to check the combined model quantitatively with the results of Carter and Bir, the sizes of the various components of the model must be estimated. The total length of each pass of the reactor was approximately $L_i = 115$ in. and the tube diameter was $d_t = 5/16 = 0.312$ in. Between the injection and measurement points there were essentially twelve passes, each of which had two 90 deg. bends.

Values of the group D/ud_t for straight pipe have been correlated as a function of Reynolds number by Levenspiel (*6*) and are shown as the dashed line in Figure 2. As mentioned above, there is no information available on mixing in 90 deg. bends, and so $L_{b\ eq}$ cannot be determined a priori. It was found that a value of

$$\frac{L_{b\ eq}}{L} = \frac{L_{b\ eqi}}{L_i} = 0.07$$

which when substituted into Equation (12) yields

$$\frac{D_e}{ud_t} = 0.93\frac{D}{ud_t} + 0.9 \qquad (13)$$

gave results of the correct order of magnitude as shown by a comparison of the solid line with the data points in Figure 2. This value in terms of pipe diameters is

$$\frac{L_{b\ eqi}}{d_t} = 26$$

or

$$L_{b\ eqi} = 8 \text{ in.}$$

This figure seems to be of an acceptable order of magnitude, since reference *1* states that systems with very roughly comparable degrees of flow disruption require about 20 to 30 pipe diameters before attempting to use an orifice flow measurement device. This length of pipe is necessary if the disturbed flow is not to cause errors in the orifice measurement. The measurement case is not directly equivalent to the mixing and dispersion problem, but it does indicate something about the order of magnitude of flow disruptions.

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Chemical Engineering—Volume I, J. M. Coulson and J. F. Richardson. (Second Revised Edition). Macmillan, New York (1964). 492 pages.

This is the first major revision of the well-known text which was first published in 1954. The total number of chapters has remained unchanged although the text has been expanded by over one hundred pages. The chapter headings are the same and cover the unit operations of fluid flow, heat and mass transfer, and combined heat mass and momentum transfer in boundary-layer and pipe flow. A final chapter on humidification operations is included.

The authors have responded to the increased emphasis of the past ten years upon fundamentals of transport processes with expanded material in these areas. There is now a more obvious recognition that fluids in motion possess momentum as well as energy, and some material on rotational flow and other fluid dynamical concepts has been included; however, there is relatively little on fluid dynamics as such, and not enough to satisfy the instructor who would like to introduce fluid dynamics in a systematic way. Increased emphasis is given to unsteady state heat transfer as well as other unsteady state processes. The material in the chapter on design applications has been expanded considerably.

The first part of the present mass transfer chapter is almost identical to that of the first edition. For those who are used to the Bird, Stewart, and Lightfoot approach to defining diffusivity, the approach here will be unsatisfactory. For example, how one would apply the relative velocity convection correction in the case of an arbitrary catalytic surface reaction is unclear. The only cases discussed are those of equal-molal counter diffusion and diffusion through a stagnant gas. For these reasons this chapter is still weak. New material on mass transfer in turbulent fluids, unsteady state mass transfer, and various mass transfer models has been added. The two-film model, penetration theory, and random surface renewal theory are discussed to some extent.

The chapter entitled, "Momentum, Heat and Mass Transfer," contains additional material on transport fundamentals and analogies; it lacks material and illustrative problems concerning simultaneous heat, mass, and momentum transfer.

The chapter on boundary layers is still good as far as it goes. By taking the integral approach exclusively, it gives no real indication of the extent of applicability of boundary-layer theory. There is no indication as to how boundary-layer theory would be used on surfaces with pressure gradients. Boundary-layer mass transfer is given short shrift; there *is* no discussion of boundary-layer transfer with chemical reaction or interaction of heat and mass transfer, as in transpiration cooling, which has become an important area for chemical engineers.

The problems are given at the end of the book rather than after individual chapters. They have been expanded to about 150 problems. Their utility has been increased by keying the problem numbers to the particular chapter involved. One of the strong points of this book has been the illustrative problems that are worked out in the text; these are as good as ever and better in some cases. This book will continue to be a valuable text for those who want an introduction to chemical engineering from the viewpoint of the unit operations, for it now includes more material on the fundamentals of the physical processes involved. Those who need a text for a course which combines both the unit operations and applications to design as well as some fundamentals of transport processes will find this book useful and valuable.

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Cryogenics, M. McClintock, Reinhold Publishing Corporation, New York (1964). 270 pages. $10.75.

This book is mainly for the nonspecialist who wishes to obtain a broad view of this important and rapidly developing field. It is descriptive in its treatment, with a minimum of mathematical equations. It is concerned largely with the physics of low-temperature phenomena and touches very briefly on the engineering aspects.

The first chapter reviews the general principles of the various methods of producing refrigeration at temperatures below −150°C. The second chapter treats the principles of thermal insulation and illustrates them by showing how various vessels, both large and small, for the storage of cryogenic liquids are insulated against heat leak from surroundings. Chapter 3 considers the various methods that are available for the measurement of low temperatures.

The next five chapters deal with the properties of materials at cryogenic temperatures. Chapter 4 describes the unusual and interesting properties of liquid helium 3 and helium 4 and discusses the theories proposed to explain these phenomena. Chapter 4 is concerned with the mechanical properties

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The effect of surface tension on factors in boiling heat transfer, Roll, John B., and John E. Myers, **A.I.Ch.E. Journal, 10,** No. 4, p. 530 (July, 1964).

Key Words: Surface Tension-6, Surface Active Agent-4, Boiling-8, Heat transfer-8, Nucleation-7, Bubbles-7, Bubble Volume-7, Growth Time-7, Delay Time-7, High-Speed Photography-10, Tween-4, Aerosol-4, Hyonic-4.

Abstract: High-speed photography has been used to record the effects of surface tension reductions on the growth and departure characteristics of bubbles in boiling heat transfer. A model is presented to describe the manner in which surface tension has an effect upon the bubble volume, delay time, and growth time. Results obtained with this model show that surface tension is effective because it changes the nucleating properties of the liquid and not because it alters its hydrodynamic character.

Solution of the equations of change by Galerkin's method, Snyder, L. J., T. W. Spriggs, and W. E. Stewart, **A.I.Ch.E. Journal, 10,** No. 4, p. 535 (July, 1964).

Key Words: Trial Functions-1, Velocity Profiles-2, Pressure Profiles-2, Temperature Profiles-2, Concentration Profiles-2, Flow or nonflow Systems-5, Fluid Dynamics-8, Heat Transfer-8, Diffusion-8, Mass Transfer-8, Boundary Value Problems-8, Initial Value Problems-8, Approximate Analysis-10, Numerical Analysis-10, Regression Analysis-10.

Abstract: The Galerkin method is adapted to the solution of the equations of change for time-dependent processes. The method uses trial functions to represent the dependent variables and yields approximate solutions in equation form. The convergence of the method is demonstrated by solving a nonlinear fluid flow problem in which inertial effects are significant.

Turbulent film condensation, Lee, Jon, **A.I.Ch.E. Journal, 10,** No. 4, p. 540 (July, 1964).

Key Words: Turbulent Heat Transfer-6, Condensation-8, Liquid Metals-10, Boundary Layer-8, Heat Transfer Coefficient-7, Reynolds Number-6, Film Thickness-9, Eddy Transport Coefficients-10, Turbulent Velocity Profile-10, Nusselt's Model-10.

Abstract: A turbulent film condensation problem was formulated. The physical model and simplifying assumptions are the same as those of Nusselt's original investigation, with the exception of including the effect of turbulent transports. The result agrees with the qualitative results of both Seban and Lee but does not agree with Dukler completely.

Prediction of efficiencies and mass transfer on a stage with multicomponent systems, Toor, H. L., **A.I.Ch.E. Journal, 10,** No. 4, p. 545 (July, 1964).

Key Words: Multicomponent Systems-8, Stage Efficiencies-8, Tray Efficiencies-8, Plate Efficiencies-8, Distillation-8, Extraction-8, Interphase Transfer-8, Mass Transfer Coefficient Matrix-1, Transfer Unit Matrices-2, Matrix Methods-10.

Abstract: Application of the linearized theory of multicomponent mass transfer to equilibrium stage devices in which the concentration changes and total flux are small shows that the composition change of each component on a stage is given by a matrix generalization of the equation for the composition change in a binary system. Composition changes depend upon the characteristic transfer units of each phase, the diffusion coefficient matrix of each phase, flow rates, and equilibrium constants. Multicomponent stage efficiencies may differ greatly from binary efficiencies.

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The calculations were based on using the constant value of $L_{b\ eq} = 0.075$ which gives only a crude estimate of the total dispersion. Obviously the amount of mixing would be a function of the flow rate but, as stated above, this type of information is not available. From further experimental work correlations of this type could be developed for use in the many cases where return bends are used. By combining these results with information for straight pipes, the mixing characteristics of any possible combination of straight and return bend sections could be predicted for design purposes.

NOTATION

C = concentration of tracer
C_o = concentration at inlet of system
C_p = concentration in straight pipe section
C_b = concentration in backmix section
D = axial dispersion coefficient for straight pipe
D_e = effective axial dispersion coefficient for entire system
d_t = pipe diameter
L = total length
L_p = length of straight pipe section
$L_{b\ eq}$ = equivalent length of backmix section
n = number of sections in total system
t = time
u = mean fluid velocity
V_b = volume of backmix section
v = volumetric flow rate
x = axial position
μ_p = p^{th} moment about origin (dimensionless)
σ^2 = variance (dimensionless)
Δ = difference between outlet and inlet moments

Subscripts

i = i^{th} section

LITERATURE CITED

1. "Fluid Meters—Their Selection and Installation," Am. Soc. Mech. Engrs. Research Publication (1933).
2. Aris, R., *Chem. Eng. Sci.*, **9**, 266 (1959).
3. Bischoff, K. B., *Can. J. Chem. Eng.*, 41, 129 (1963).
4. Carter, D., and W. G. Bir, *Chem. Eng. Progr.*, **58**, 40 (1962).
5. Cholette, A., and L. Cloutier, *Can. J. Chem. Eng.*, **37**, 105 (1959).
6. Levenspiel, O., *Ind. Eng. Chem.*, **50**, 343 (1958).
7. ———, *Can. J. Chem. Eng.*, **40**, 135 (1962).
8. ———, and W. K. Smith, *Chem. Eng. Sci.*, **6**, 227 (1957).
9. ———, and K. B. Bischoff, in "Advances in Chem. Eng.," vol. 4, (1963).
10. May, W. G., *Chem. Eng. Progr.*, **55**, 49 (1959).
11. Van der Laan, E. T., *Chem. Eng. Sci.*, 7, 187 (1958).