u = unmeasured components of v
m = measured components of v
F, G, H, J, K, M, P, R = matrices defined by (2.1) to (2.3)
R^+ = generalized inverse of R
$\mathcal{R}$ = error free (actual) model matrix, R
E = error matrix ($R = \mathcal{R} + E$)
b = $y - Qm$
$\sup_x$ = supremum over all x
S = diagonal matrix of reciprocal standard deviations of ϵ
ϵ = noise component of b
$DP(i, j)$ = normalized dot product of vectors r_i, r_j defined by (2.9)
Γ = distortion matrix given by (4.4)
$\mathcal{E}^\circ(t)$ = local transient error $= \dot{x}(t) - Jd^\circ(t)$
$\mathcal{E}(u)$ = global transient error given by (4.9)

Superscripts

$\wedge$ = denotes vector or matrix which has been reduced by selecting certain elements from the original quantity
-1 = inverse
$+$ = generalized inverse

Subscripts

e = denotes estimated quantity
m = denotes measured quantity

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A Mathematical Model for Heat Transfer in a Packed Bed and a Simplified Solution Thereof

Heat transfer in packed beds can be mathematically modeled to account for the heat transfer between the particles and the gas phase, the conduction through the solid phase of particles, and the mixing or dispersion within the gas phase in the void structure of the porous media. To solve the resulting differential equations numerically is not easy. The solution for sinusoidal gas temperature input assumes linearity of the logarithm of the temperature with time. If, in addition, linearity with distance can be assumed, then the solution can be vastly simplified to finding the real root of a fourth-order algebraic equation.

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SCOPE

Our research in porous media was originally directed toward the elucidation of the heat transfer between the gas phase and the particles in a fluidized bed system; this was to be accomplished by frequency response methods. In order to understand the fluidized bed system it was first necessary to investigate the heat transfer characteristics of the packed bed system and to consider all the effective modes of transfer of heat that are known or suspected to occur. It is well known that the heat transfer coefficient from the particle to the gas phase cannot be established without assuming some mathematical model for the process. The coefficient depends upon the model assumed. In any adequate model there will usually be several adjustable parameters that describe the pysical attributes of the system. Unfortunately, models that are

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adequate usually involve difficult numerical solutions, and these must be accomplished a large number of times until the adjustable parameters are such that the solution fits the experimental data. Any means of reducing the complexity of the solution and the time involved in obtaining the parameters would be helpful. It is to these points that the present work is addressed.

The model for the description of the heat transfer in a packed bed has been developed independently by Brodkey (1964) and Kim (1965) and by Barile (1966) and has been presented in detail by Littman et al. (1968). These latter authors solved the complete set of equations for sinusoidal gas temperature inputs. Because of the complexity of the method, the three adjustable parameters were not completely established from the frequency response data. The parameters associated with the dispersion was taken from the literature and not established from the frequency response data. This simplified the analysis considerably since only two parameters had to be fitted. More recently Littman and Sliva (1970) obtained data at low Reynolds numbers for which the dispersion literature data were not available; consequently, although considerably more complex, they did fit all three parameters.

Two recent papers should be mentioned. Turner (1967) discussed the model used here to find the adjustable parameters. His analysis was based upon the solution of the equations using experimental data directly (3 points to determine the three parameters) rather than an optimum fit to any amount of data. Unfortunately such data are not accurate enough for this to be easily accomplished. More recently Lindeaur (1967) used the frequency response method to determine the heat transfer coefficient, but because he used high enough Reynolds numbers he did not need to consider the dispersion in his experiments.

CONCLUSIONS AND SIGNIFICANCE

The model descriptive of the heat transfer in a packed bed is referred to as the conduction-dispersion model. It considers the heat transfer between the particles and the gas phase, the conduction through the solid phase of particles, and the mixing or dispersion within the gas phase in the void structure of the porous media. The energy conservation equation and assumed boundary conditions completely define the system. The resulting differential equations, which are equivalent to a linear fourth-order partial system, can be solved for sinusoidal inputs and the assumed boundary conditions. The numerical solution is not simple since it involves a system of eight linear, complex-coefficient, algebraic equations in eight unknowns. A solution was achieved by Littman et al. (1968) by a numerical matrix inversion method which consisted of an adaptation to complex matrices of the Gauss-Jordan method with pivotal selection.

The solution described above assumes linearity of the logarithm of the gas temperature with time. If in addition, experimental observations are used to establish the linearity of the system with respect to distance, then the solution can be vastly simplified to finding the real root of a fourth-order algebraic equation. Furthermore, under these conditions there is no need for boundary conditions and the solution is very simple. For this to be valid, it is sufficient to show that the measured gas temperature waves are sinusoidal and have identical frequencies regardless of the location in the bed and that the amplitude ratio and phase shift of the waves at any two points at a given frequency are dependent only on the relative vertical displacement. The complete solution of the differential equation offered by Littman does require the first experimental observation but does not necessitate the latter. In the range of our experiments the latter experimental observation was also valid (Kim, 1965). Only in the low Reynolds number range of the results of Littman and Sliva (1970) does the approximation fail, and the complete solution should be used.

FREQUENCY RESPONSE METHOD

The successful and extensive application of frequency response methods for the characterization of the time dependency of complex electronic networks is well known. However, the application to the characterization of flow systems, where the additional effect of location is involved, is relatively new. Even so, this method has been used to investigate a number of transfer problems in chemical engineering research. In this method, a signal of a certain amplitude and frequency is impressed on the system under investigation. The resulting output signal from the system has a damped amplitude and has a phase shift but with the same frequency. The signal can be any physical quantity which corresponds to a driving force. The ratio of the two amplitudes and the phase shifts at various frequencies can be used to evaluate the differential equation (or transfer function) which represents the system. When the differential equation is linear, the ratio and phase shifts are functions of the frequency only and can be used for the selection of the proper differential equation or to determine the coefficients that are descriptive of the system or both. The frequency response method is ideal for the study of the heat transfer in a packed bed where three mechanisms are potentially important. It allows the adequate selection of the differential equation and evaluation of the descriptive parameters. Consequently, its use has found application to the transfer problem in packed and fluidized beds. Littman and his co-workers used a shark-fin shaped imput and studied the first few harmonics of the output wave. In contrast, in our work we superimposed a sinusoidal wave and studied the amplitude decay and phase shift as a function of the frequency.

METHOD OF SOLUTION

The basic pair of differential equations resulting from the conduction-dispersion model are

$$\alpha_g \frac{\partial U}{\partial \theta} + \frac{\partial U}{\partial x} - \gamma_g \frac{\partial^2 U}{\partial x^2} = -\phi_L(U - V) \qquad (1)$$

$$\phi_L \frac{\partial V}{\partial \theta} - \gamma_s \phi_L \frac{\partial^2 V}{\partial x^2} = -\phi_L(V - U) \qquad (2)$$

For the simplified method of solution undertaken here, the boundary conditions which have to be assumed for the numerical solution are not needed and thus are not presented.

Since the gas temperature is assumed to be linear with respect to time and vertical distance, it can be expressed as the product of a rotating unit vector and a distance dependent vector

$$U = A(x)\, e^{i\eta\theta} \tag{3}$$

Since the coefficients are assumed to be constant, the solid temperature may also be expressed as

$$V = B(x)\, e^{i\eta\theta} \tag{4}$$

Combining Equations (3) and (4) into the pair of differential equations (1) and (2) and differentiating with respect to time, there results a pair of equations

$$-\gamma_g \frac{d^2A}{dx^2} + \frac{dA}{dx} + (\phi_L + i\alpha_g\eta)A = \phi_L B \tag{5}$$

$$\gamma_s \frac{d^2B}{dx^2} - (1 + i\eta)B = -A \tag{6}$$

The variable B can be eliminated between Equations (5) and (6) to give a fourth-order, linear, ordinary differential equation with constant but complex coefficients

$$\frac{d^4A}{dx^4} - \frac{1}{\gamma_g}\frac{d^3A}{dx^3} - \left(\frac{\phi_L}{\gamma_g} + \frac{1}{\gamma_s}\right) + i\left(\frac{\alpha_g\eta}{\gamma_g} + \frac{\eta}{\gamma_s}\right)\frac{d^2A}{dx^2} + \left(\frac{1}{\gamma_s\gamma_g}\right) + i\left(\frac{\eta}{\gamma_s\gamma_g}\right)\frac{dA}{dx} + \left(-\frac{\eta^2\alpha_g}{\gamma_s\gamma_g}\right) + i\left(\frac{\eta\alpha_g + \eta\phi_L}{\gamma_s\gamma_g}\right)A = 0 \tag{7}$$

At this point the normal procedure would be to solve the equation in the manner as accomplished by Littman et al. (1968). The true form of the solution must be

$$U - U_0 = \left\{ \sum_{i=1}^{4} C_i\, e^{-(K_i + i\,\Phi_i)x} \right\} e^{i\eta\theta} \tag{8}$$

that is, the amplitude $A(x)$ of Equation (3) or A of Equation (7) is the sum of four terms given in the brackets of Equation (8). The experimental results suggest that this is more complex than necessary and that an adequate representation can be obtained by using just one term of the series, that is, three of them are negligible. Thus, the solution is assumed to be

$$A(x) = C\, e^{-(K + i\,\Phi)x} \tag{9}$$

The values of K and Φ must be identical to the corresponding experimental values within the experimental error, if the assumed model is correct. The substitution of this solution into Equation (7), differentiating with respect to the vertical distance x, and cancellation of the gas amplitude term C results in

$$m^4 - \frac{1}{\gamma_g}m^3 - \left\{\left[\frac{\phi_L}{\gamma_g} + \frac{1}{\gamma_s}\right] + i\left[\frac{\eta\alpha_g}{\gamma_g} + \frac{\eta}{\gamma_s}\right]\right\}m^2 + \left(\frac{1}{\gamma_s\gamma_g}\right) + i\left(\frac{\eta}{\gamma_s\gamma_g}\right)m + \left(-\frac{\eta^2\alpha_g}{\gamma_s\gamma_g}\right) + i\left(\frac{\eta\alpha_g + \eta\phi_L}{\gamma_s\gamma_g}\right) = 0 \tag{10}$$

where

$$m = -(K + i\,\Phi) \tag{11}$$

The equation can be separated into the real and imaginary parts. For the complex identity, the real part becomes

$$\gamma_g\gamma_s(K^4 + \Phi^4 - 6K^2\Phi^2) + \gamma_s(K^3 - 3\Phi^2)K - (\gamma_g + \phi_L\gamma_s)(K^2 - \Phi^2) + (\gamma_g + \alpha_g\gamma_s)2K\Phi\eta - K + \eta\,\Phi - \alpha_g\eta^2 = 0 \tag{12}$$

and the imaginary part is

$$4\gamma_g\gamma_s(K^2 - \Phi^2)K\,\Phi + \gamma_s(3K^2 - \Phi^2)\,\Phi - (\gamma_g + \phi_L\gamma_s)2K\,\Phi - (\gamma_g + \alpha_g\gamma_s)(K^2 - \Phi^2)\eta - \Phi + \eta K + (\alpha_g + \phi_L)\eta = 0 \tag{13}$$

Finally the two equations can be most easily solved for the frequency dependent term η and equated. This results in a fourth-order, algebraic equation which relates the parameters descriptive of the heat transfer from the particle to the gas (ϕ_L), the conduction through the particle phase ($\gamma_s\phi_L$), and the mixing in the gas phase (γ_g). The adequacy to which such a model can represent the experimental data depends first upon the adequacy of the model, and second on the adequacy of the approximation which involved the assumptions of the linearity of the logarithm of the gas temperature with respect to both time and vertical distance. For these later assumptions to be valid it is sufficient to show that the measured gas temperature waves are sinusoidal and have identical frequency regardless of location in the bed and the amplitude ratio and phase shift of the waves at any two points at a given frequency are dependent only upon the relative vertical displacement. Both the approximate and complete solution of the differential equations requires the first of these two experimental observations, but the complete solution does not necessitate the latter although the approximate solution does. In our experimental work this latter assumption was valid although at very low Reynolds numbers it is not true as determined from some of the work of Sliva (1968).

The solution of the fourth-order, algebraic equation involves a simple trial and error iteration. The three adjustable parameters, (ϕ_L, $\gamma_s\phi_L$, γ_g) could be obtained by curve fitting of the amplitude ratio and phase shift data to the theoretical estimates. We accomplished this by using an optimization program. With initial guesses of the parameters, the optimization routine determined the optimized final values which gave the best fit of the predicted phase shift and amplitude ratio decay when compared to the actual reported experimental data.

Other simpler models can be easily obtained from the present formulation by setting one or more of the characteristic parameters to zero. In our formulation these will be approximate solutions except under conditions of only one characteristic parameter, that is, heat exchange between particle and gas only or axial dispersion of mass in a bed without small scale pores. Under these conditions, the basic equation is first-order and our approximation is exact.

RESULTS

The conduction-dispersion model is the most complex model that has been used to describe the heat transfer in the packed bed system. Littman et al. (1968) has shown the adequacy of the model. Our purpose here is to present the simplified solution of the resulting differential equations. In effect we are testing the approximation of the simplified solution, although the assumption is often justified by the data itself. In addition, because of the optimization technique involved, the best possible values of the descriptive coefficients are determined without regard to visual curve fitting techniques that had been previously used to provide the best values. The latter method often introduces bias since unreasonable values are easily rejected. However, experimental data that are poor or do not fit the model can lead to unreasonable values in order to get the best fit by optimization.

We are more concerned here with a comparison between the numerical results of Littman et al. (1968) and the approximate solution with optimization rather than with detailed comparisons of data and correlations of that data. Probably the recent article by Kato and Wen (1970) is the best for this latter purpose.

The present procedure in no way changes the conclusions reached by Littman et al. (1968). It does, however, raise the question of the reliability of some of the data which are recognized as most difficult to obtain and which often require corrections to account for the heat transfer to the supporting screen at the inlet. In this respect, one can learn much from the detailed comparison of the ampli-

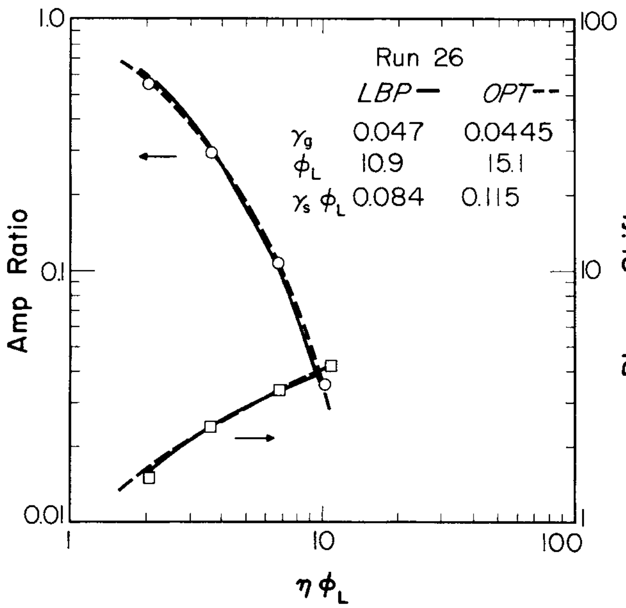

Fig. 1. Amplitude ratio and phase shift comparison (Run 26).

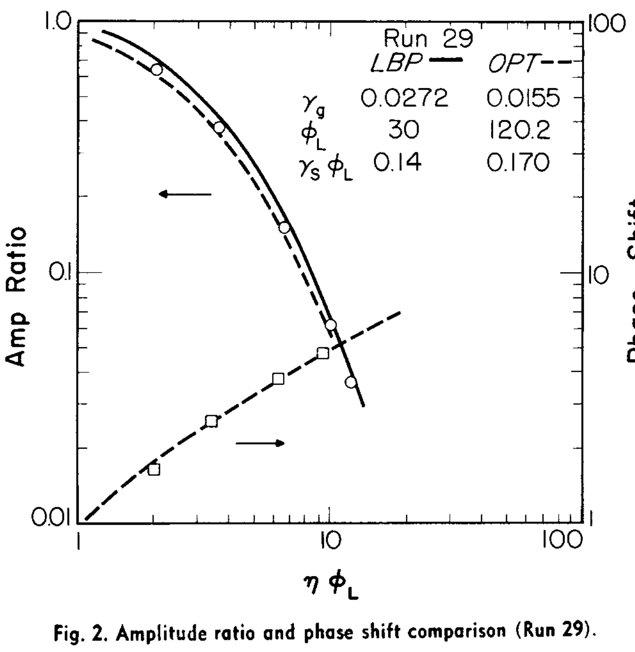

Fig. 2. Amplitude ratio and phase shift comparison (Run 29).

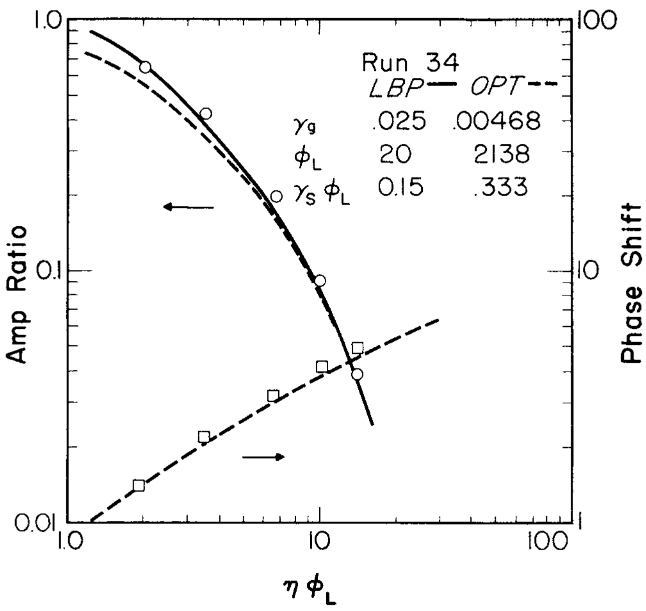

Fig. 3. Amplitude ratio and phase shift comparison (Run 34).

tude ratio (AMP RATIO, outlet to inlet) and phase shift (in radians) versus the dimensionless frequency parameter. Figure 1 gives the results of one of the more successful runs where the data, the numerical solution, and the optimization results are all compared. Both are adequate fits, and the differences in the descriptive parameters are small showing that the approximate solution is indeed adequate, at least for this region of parameter values. Figure 2 is another completely satisfactory fit. Of importance here is the relative insensitivity of the curve to two of the parameters in this range. Accurate evaluation of the parameters would require experimental accuracy far beyond presently available. In contrast, Figure 3 shows a run where the optimization does not fit the data adequately. Either the data are inadequate, the basic three parameter model is unsatisfactory, or the assumption in the approximate solution is not valid. There are over 50 runs where such comparisons were made and the majority gave excellent comparisons as in Figures 1 and 2. The inadequate ones included some that were in the original data tabulations (Barile, 1966; Sliva, 1968) but were of enough question that they were not evaluated by the authors.

Figures 4 and 5 provide a direct comparison between the complete solution and the simplified solution for the given parameters. Only for very large values of the parameter $\gamma_s\phi_L$ is there an appreciable difference.

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NOTATION

A = a function of x
A_c = cross-sectional area of column
A_p = surface area of particles/unit length of bed
B = a function of x
C_g = specific heat of gas
C_s = specific heat of particles
D_p = particle diameter

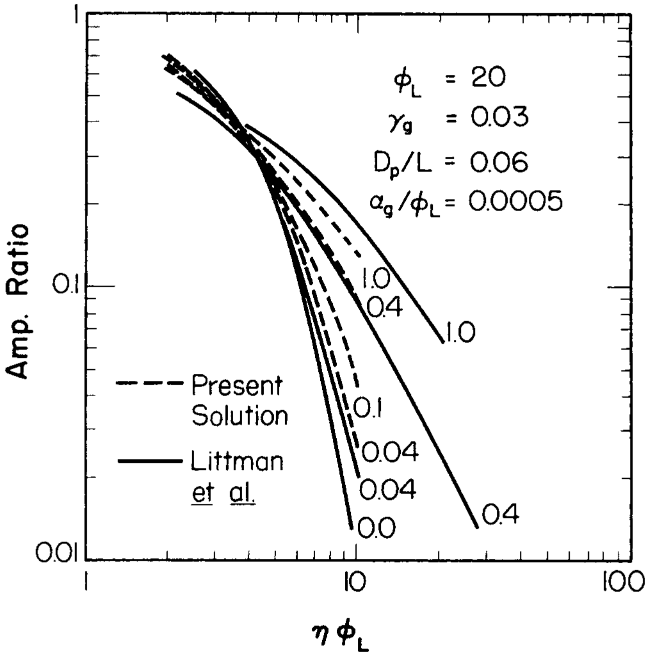

Fig. 4. Amplitude ratio by exact and approximate methods.

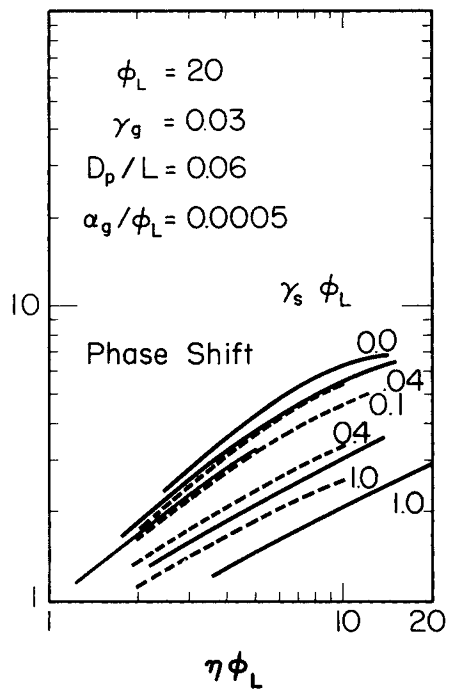

Fig. 5. Phase shift by exact and approximate methods.

G = mass flow rate of gas
h = gas-particle heat transfer coefficient
k_{eg} = effective thermal conductivity of gas phase
k_{es} = effective thermal conductivity of solid phase
k_{e0} = stagnant bed conductivity
k_g = molecular conductivity of the gas
k_s = molecular conductivity of the solid particle
L = bed length
q = interphase heat transfer rate
S = bed weight/unit length of bed
T = temperature
T_{go} = average temperature of inlet or outlet temperature wave
t = time
U = dimensionless gas temperature $= \dfrac{T_g - T_{go}}{\alpha\, T_{go}}$
V = dimensionless solids temperature $= \dfrac{T_s - T_{go}}{\alpha\, T_{go}}$
v_g = volumetric flow rate of gas
x = z/L
z = column height variable

Greek Letters

αT_{go} = amplitude of sinusoid
α_g $= \dfrac{\gamma L}{v_g} \dfrac{\omega}{\eta}$
γ = void volume per unit length of bed
$\gamma_s \phi_L$ $= \dfrac{k_{es} A_c (1 - \epsilon)}{v_g \rho_g C_g L}$
γ_g $= \dfrac{k_{eg} A_c \epsilon}{v_g \rho_g C_g L}$
ϵ = void fraction
η $= \dfrac{SLC_s\omega}{hA_pL}$
$\eta\phi_L$ $= \dfrac{SLC_s\omega}{v_g\rho_g C_g}$
θ $= \dfrac{\omega t}{\eta}$
μ_g = gas viscosity
ρ_g = gas density
ϕ_L $= \dfrac{hA_pL}{v_g\rho_g C_g}$
ω = angular velocity

Subscripts

s = solid particle
g = gas

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