TRANSIENT HEAT AND MASS TRANSFER IN AN ADIABATIC REGENERATOR—A GREEN'S MATRIX REPRESENTATION

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Abstract—A mathematical model is proposed which describes transient heat and mass transfer within a porous medium with bulk flow in an adjacent channel. This physical process is descriptive of regenerative type mass exchangers in which a solute is removed from a fluid phase by sorption onto the internal surface area of a porous material.

An integral formulation of the solution to the mathematical model in terms of the Green's functions is presented. Once the Green's functions are determined the solution to the problem for any arbitrary inlet, initial and boundary condition is readily obtained by evaluating integrals involving the Green's functions and the known conditions. The solution to the mathematical problem for the case in which generation of heat and mass occurs within the porous material can also be written down immediately as an integral involving the Green's functions and the known functions describing the generation of heat and mass.

For the special case where resistance to heat and mass transfer between flowing phase in the channel and external surface of the porous medium is negligible, the Green's functions are determined in the Laplace domain of the time variable. Using these Green's functions exact solutions are obtained for constant initial conditions and step change inputs at the inlet. These solutions allow calculation of temperature and concentration profiles within the porous material itself. Such complete solutions to similar problems have not previously been reported in the literature. These solutions are in the form of improper integrals, which are best evaluated using a digital computer.

It was found that the breakthrough curves for the adiabatic mass exchanger actually exhibit two breakthroughs in contrast to the single breakthrough exhibited by the isothermal mass exchanger.

 C_{Iii}

NOMENCLATURE

- A, matrix of constants defined by equation (47);
- a, $\operatorname{cross\,sectional\,area\,of\,channel}\left[\operatorname{cm}^{2}\right];$
- a_i , diagonal elements of $-\Lambda$;
- A_k , functions defined by equation (77);
- B, matrix of constants defined by equation (44);
- B_1 , function defined by equation (79);
- B_2 , function defined by equation (80);
- C, concentration of diffusing species in gas phase $[g/cm^3]$;
- C_c , solute concentration in the channel [g/cm³];

functions defined by equation (76);

 C_{p} , heat capacity of matrix [cal/g °K]; C_{pg} , heat capacity of fluid phase [cal/g °K]; °K];

C_r concentration about which equilibrium relationship is linearized [g/ cm³];

$$C_{Rij}$$
, functions defined by equation (75);

D, molecular diffusivity $[cm^2/s]$; F_n dimensionless generation ter

- dimensionless generation terms of mass and heat in equations (31) and (32);
- functions defined by equation (72);
- 4×4 array of Green's functions; where indicated, 2×2 submatrix of Green's functions;

 f_{ij} G.

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- g, diffusion coefficient corrective factor for porous medium which allows for the fact that diffusion is not along a straight path, dimensionless;
- G_{ij} , elements of the Green's function matrix;
- H, matrix defined by equation (48);
- h_E , heat transfer coefficient between channel and porous material interface [cal/s cm² °K];
- h_M , mass transfer coefficient between channel and porous material interface [cm/s];
- K, Henry's law type equilibrium constant, dimensionless;
- k, effective thermal conductivity of the bulk porous medium,

 $k + [\varepsilon/(1 - \varepsilon)] k_g [\text{cal/s cm }^\circ\text{K}];$

$$(1 - c)k + ck \int cal/s cm {}^{\circ}K$$

- $(1 \varepsilon) k_s + \varepsilon k_g [\text{cal/s cm }^{\circ} \text{K}];$ k_g, thermal conductivity of fluid phase [cal/s cm $^{\circ} \text{K}$];
- k_s , thermal conductivity of non-fluid phase [cal/s cm °K];
- K_t , temperature coefficient of sorption equilibrium,

$$-\left.\rho_{p}\frac{\partial\Gamma}{\partial T}\right|_{c_{0},T_{0}}\left[g/cm^{3}\,^{\circ}\mathrm{K}\right]$$

- L, thickness of porous material in y_A direction [cm]; matrix differential operator defined by equations (12)-(15);
- \tilde{L} , adjoint differential operator defined by equations (17)–(20);
- Le, dimensionless parameter,

$$c_{na} g D \varepsilon / k_{ch};$$

- m_{ijk} , three dimensional array of 8 components whose real and imaginary parts are defined by equations (89)-(101);
- Nu, Nusselt number, $h_E L/k_{ch}$, dimensionless;
- P, constant decoupling matrix defined by equation (55);
- p, active perimeter of channel [cm];

- *Pe*, Peclet number, *av/pegD*, dimension-less;
- Q, matrix of constants defined by equation (61);
- q, heat of sorption [cal/g];
- R, matrix of constants defined by equation (64);
- r_{i} , the characteristic roots of the matrix $[-(1 \lambda \gamma) A]$, defined by equations (53) and (54);
- s, Laplace transform parameter;
- Sh, Sherwood number, $h_M L/\epsilon gD$, dimensionless;
- T, temperature [°K];

t, dimensionless time,

$$gDt_A/[\varepsilon + (1 - \varepsilon)K]L^2;$$

- substitution for τt ;
- t_A , time [s];

ť,

- T_c , temperature of fluid phase in the channel [°K];
- U, dependent vector whose components U_1, U_2, U_3, U_4 represent dimensionless concentration and temperature within the porous material and in the channel; dependent subvector U_1 , U_2 ;
- U_1 , dimensionless fluid phase solute concentration within the porous material, C/C_0 ;
- U_2 , dimensionless temperature within the porous material, T/T_0 ;
- U_3 , dimensionless solute concentration in the channel, C_c/C_0 ;
- U_4 , dimensionless temperature in the channel, T_c/T_0 ;
- U_3^0, U_4^0 , constant dimensionless concentration and temperature at the inlet;
- v, gas velocity through the channels [cm/s];
- V_{iR} , functions defined by equation (84);
- V_{il} , functions defined by equation (85);
- x, dimensionless coordinate in direction of flow, x_A/LPe ;
- x', substitution for ξx ;
- x_A , coordinate in direction of gas flow (zero at gas inlet) [cm];

 k_{ch}

- y, dimensionless coordinate in the direction of diffusion, y_A/L ;
- y_A , coordinate in the direction of diffusion [cm];
- Z_1 , complex quantity defined by equations (82) and (83);
- Z_2 , branch of $\sqrt{(Z_1)}$ defined by equation (81).

Greek symbols

α, generalized Lewis number for the porous medium,

$$\frac{\varepsilon + (1 - \varepsilon) K}{\varepsilon g D} \cdot \frac{k}{\rho_p c_p + K_t q};$$

- Γ, equilibrium composition of solute on sorbent, g solute/g sorbent;
- $\tilde{\Gamma}$, dimensionless equilibrium relationship such that

 $\rho_p \Gamma = \text{constant} + KC - K_t T;$

 φ, dimensionless parameter which is a measure of the effect of concentration changes on temperature,

$$\frac{qK}{\rho_p C_p + K_t q} \cdot \frac{C_0}{T_0};$$

 $\delta(x)$, Dirac delta function;

 δ_{ij} , Kronecker's delta;

- ε, porosity of the matrix, vol. voids/ total vol., dimensionless; arbitrary positive number used in limit expressions;
- η , dimensionless coordinate in the direction of diffusion, same as y;
- Λ , diagonal matrix whose diagonal is $-a_1$ and $-a_2$;
- λ , dimensionless parameter which is a measure of the effect of temperature changes on concentration,

$$\frac{(1-\varepsilon)K_t}{\varepsilon+(1-\varepsilon)K}\cdot\frac{T_0}{C_0};$$

- ξ , dimensionless longitudinal coordinate, same as x;
- $\rho_g,$ density of fluid phase [g/cm³];

- $\begin{array}{ll} \rho_{p}, & \text{mass of sorbent per unit vol. of solid} \\ & \text{phase } [g/\text{cm}^{3}]; \\ \tau, & \text{dimensionless time, same as } t; \\ \varphi_{R}, & \text{function defined by equation (73);} \\ \varphi_{I}, & \text{function defined by equation (74);} \end{array}$
- Ψ , transformed matrix of Green's functions, *PG*.

INTRODUCTION

THIS paper presents solutions to the system of partial differential equations describing unsteady state simultaneous heat and mass transfer in porous media. These partial differential equations are descriptive of the physical process occurring in adiabatic regenerator type mass exchangers where a solute is sorbed from an inactive carrier gas onto the internal surface area of a porous material. The essential feature of the process regardless of the exact geometry is that mass and heat transfer due to diffusion and conduction occur in a region different from the flowing fluid phase, where mass and heat transport is due primarily to convection.

In designing regenerator type mass exchangers one is usually interested in the so-called breakthrough curves, that is, the time response of the effluent stream solute concentration to the input concentration. In 1952 Rosen [1] obtained a solution for the isothermal case in which a solute is sorbed internally within spherical particles from a gas phase passing in bulk flow through the bed of particles. By assuming a linear equilibrium relationship between solute in the fluid phase and sorbed phase Rosen obtained an analytical solution for the breakthrough curve as a real integral which was then evaluated numerically. The essential feature of Rosen's model is that mass transfer within the porous particle is described in terms of a diffusion process. Rosen's model also allows for resistance between the bulk fluid phase outside the particles and the particle external surface by means of a constant mass transfer coefficient. Previous to Rosen's work resistance to mass transfer within the particle had also

been accounted for by means of an overall mass transfer coefficient. This model of the process gives rise to the well known Schumann-Anzelius solutions [2, 3] which have been extensively tabulated by Larsen [4]. These solutions are also well discussed in the book by Jakob [5]. Masamune and Smith [6, 7] have generalized Rosen's solutions to include a third resistance, the rate of sorption within the porous particle. Using Green's functions and matrix representation Wernick [8] presented solutions to this problem for arbitrary initial bed loading and inlet conditions. Other systems of partial differential equations handled by matrices and Green's functions are the electromagnetic equations described in Morse and Feshbach [9] and the creeping flow equations of Oseen [10].

If the process of sorption from a fluid phase within a porous material is viewed as adiabatic, the heat of sorption will cause temperature gradients within the porous materials. Since the equilibrium relationship between solute in the sorbed and fluid phase may depend strongly upon temperature as well as concentration, a coupling between the concentration and temperature profiles is established. Coupled problems in which resistance to mass and heat transfer in the direction transverse to the flow of the fluid phase is accounted for by means of overall transfer coefficients have been treated numerically by Bullock [11] and Chi [12]. Mathematically this description of the process is somewhat simpler than that in which the mechanism of heat and mass transport in the porous material is considered as a diffusional process. With overall transfer coefficients a system of four first order partial differential equations is obtained. With diffusional transport in the porous region, two second order and two first order partial differential equations are obtained.

One of the earliest treatments of two coupled linear diffusion equations appears to be that of Henry [13]. The more recent monograph of Luikov and Mikhailov [14] presents solutions to linear systems of two coupled diffusion equations for boundary conditions of first, second and third kind. Norden and David [15] have presented finite difference solutions to nonlinear systems of coupled diffusion equations arising in their studies of the drying of wool. In none of the work of these latter three groups were provisions made to account for flow of a fluid phase at the boundaries of the region in which the diffusional transport is occurring. Thus, the physical system considered in this paper is a combination of the type of process considered by the authors in the above paragraph and the type of process considered by Rosen [1].

The most general treatment of a problem involving coupled heat and mass transport by diffusion in a stationary region with convective transport in an adjacent region is the strictly numerical solution of Weber and Meyer [16] which appeared while this study was in progress. Since they solved the system of partial differential equations by finite differences they were able to handle nonlinear equilibrium relationships as well as nonconstant physical properties. Unfortunately, their solution requires prohibitively lengthy computer times. In order to keep the computer time down to a reasonable value rather large increment sizes were used; this can give rise to appreciable error. As a result of this Weber and Meyer did not explore the behavior of this system. By assuming that physical properties are constant and that the equilibrium relationship can be linearized, a linear system of four partial differential equations is obtained whose analytical solution is presented in this paper. In the next section the problem is defined mathematically and an integral representation of the solution is presented in terms of the Green's function matrix and arbitrary but known initial and inlet concentration and temperature profiles. The advantage of presenting the solution in this form is that once the Green's function matrix has been obtained the solution can be obtained for any given inlet and initial conditions in terms of integrals involving these known conditions and the known Green's functions. The effect of arbitrary but known generation terms of heat and mass may also be expressed as integrals involving these terms and the Green's function.

A special case of the solutions presented in this paper has been given previously [17]. The solution in [17] is for the case when the sorbing medium is semi-infinite in the direction transverse to the direction of flow, or alternatively, when the values of time under consideration are small. Since in [17] also no resistance to heat and mass transfer in the channel was considered, solutions to step inputs in concentration and temperature could be expressed as linear combinations of error functions. For constant generation of heat and mass in a fuel cell electrode, solutions were obtained as repeated integrals of error functions. In the present paper solutions are obtained which are good for all values of time for sorbing media of finite thickness, and a more general Green's function formulation is given.

MODEL AND ITS INTEGRAL REPRESENTATION

Consider equilibrium sorption and diffusion of a dilute species, such as water vapor, and diffusion of heat with generation in a porous medium of finite thickness with bulk flow in an



 Y_A (Y or η in dimensionless form)



adjacent channel as shown in Fig. 1. According to Henry's classical analysis of diffusion of heat and moisture in a textile fiber [13], its more recent treatment from the point of view of irreversible thermodynamics in Luikov and Mikhailov's book [14], and our previous description of the model [17–19], the coupled partial differential equations for diffusion and rapid sorption in the matrix are

$$\frac{\partial U_1}{\partial t} - \lambda \frac{\partial U_2}{\partial t} - \frac{\partial^2 U_1}{\partial y^2} = 0 \tag{1}$$

$$-\gamma \frac{\partial U_1}{\partial t} + \frac{\partial U_2}{\partial t} - \alpha \frac{\partial^2 U_2}{\partial y^2} = 0.$$
 (2)

 U_1 is the dimensionless concentration in the porous matrix and U_2 is the dimensionless temperature as defined in the Nomenclature. The dimensionless groups λ and γ are measures of the coupling between temperature and concentration. The group α involves a ratio of the thermal diffusivity to molecular diffusivity. All three groups depend upon the linearized equilibrium relationship for the diffusing substance.

The partial differential equations for the dimensionless concentration in the channel, U_3 and for the temperature U_4 are

$$\frac{\partial U_3}{\partial x} + Sh(U_3 - U_1 \bigg|_{y=0}) = 0$$
 (3)

$$\frac{\partial U_4}{\partial x} + \frac{Nu}{Le} (U_4 - U_2 \bigg|_{y=0}) = 0.$$
 (4)

Constant Sherwood and Nusselt numbers have been used to correct for any resistances to mass and heat transfer in the thin channel. In a previous publication we have shown the extent of validity of such assumption for a simple regenerator problem [20]. The group *Le* differs from the usual Lewis number principally due to the fact that the thermal conductivity involves the conductivity of the matrix as well as of the gas.

To completely determine the solution to equations (1)-(4) we must specify inlet, initial and boundary conditions. The inlet conditions are that the functions $U_3(t, 0)$ and $U_4(t, 0)$ must be given for t > 0. Initial conditions are that $U_1(0, x, y)$ and $U_2(0, x, y)$ are given for x > 0, 0 < y < 1. At y = 0 we have the boundary conditions

$$\left. \frac{\partial U_1}{\partial y} \right|_{y=0} + Sh(U_3 - U_1 \bigg|_{y=0}) = 0$$
 (5)

$$\left. \frac{\partial U_2}{\partial y} \right|_{y=0} + Nu(U_4 - U_2 \bigg|_{y=0}) = 0.$$
 (6)

These equations result from the continuity of heat and mass fluxes at the interface between the porous media and the fluid phase in the channel. A final boundary condition at y = 1must be specified. We will assume that at y = 1the porous material is impermeable to heat and mass. This implies that the dimensionless concentration and temperature gradients $(\partial U_1/\partial v)$ and $(\partial U_2/\partial y)$ be zero at y = 1. In the more general Green's function formulation that follows it is necessary to decide only whether the boundary condition is of first, second or third type. Thus we will specify the more general boundary condition of second type, that is the gradients $(\partial U_1/\partial y)$ and $(\partial U_2/\partial y)$ must be specified as functions of t and x at y = 1.

Using equations (5) and (6), equations (3) and (4) can be rearranged into

$$\frac{\partial U_3}{\partial x} - \frac{\partial U_1}{\partial y}\Big|_{y=0} = 0$$
 (7)

$$\frac{\partial U_4}{\partial x} - \frac{1}{Le} \frac{\partial U_2}{\partial y} \bigg|_{y=0} = 0.$$
 (8)

For the case where resistance to mass and heat transfer is negligible between channel fluid phase and porous material interface, i.e. Nu and $Sh \rightarrow \infty$, boundary conditions (5) and (6) become

$$U_1|_{y=0} = U_3$$
 (9)

$$U_2|_{y=0} = U_4. \tag{10}$$

This case occurs when the channel is very thin or when the diffusivities in the matrix are much lower than those in the channel.

The adjoint equations and an integral representation

A completely non-homogeneous problem for the set of partial differential equations given by equations (1)-(4) is best solved by the method of Green's functions as are all other linear non-homogeneous boundary value problems. To apply the method we must first obtain an integral theorem giving the solution to the nonhomogeneous problem in terms of Green's functions. To obtain such an integral representation, we form a divergence expression as follows:

$$(LU)^*G - U^*(\tilde{L}G) = a \text{ divergence}$$
 (11)

where U is the unknown vector, L the differential operator matrix, G the Green's function matrix, * refers to the transpose of the matrix and \sim refers to the adjoint to be constructed. Specifically let L be the operator such that L operating on the column vector U with components U_1, U_2, U_3, U_4 results in the column vector LU whose four components are

$$(LU)_{1} = \frac{\partial U_{1}}{\partial t} - \frac{\partial^{2} U_{1}}{\partial y^{2}} - \lambda \frac{\partial U_{2}}{\partial t}$$
(12)

$$(LU)_{2} = -\gamma \frac{\partial U_{1}}{\partial t} + \frac{\partial U_{2}}{\partial t} - \alpha \frac{\partial^{2} U_{2}}{\partial y^{2}} \qquad (13)$$

$$(LU)_{3} = \frac{\partial U_{3}}{\partial x} + Sh(U_{3} - U_{1}\Big|_{y=0}) \qquad (14)$$

$$(LU)_4 = \frac{\partial U_4}{\partial x} + \frac{Nu}{Le} (U_4 - U_2 \bigg|_{y=0}).$$
(15)

Let $G_{ij}(i, j = 1,2,3,4)$ be the 4×4 array of Green's functions. For the present we will consider each G_{ij} as a six place function of the three source coordinates (t, x, y) and the three observer coordinates (τ, ξ, η) , that is,

$$G_{ij} = G_{ij}(\tau, \xi, \eta; t, x, y). \tag{16}$$

We can now construct a matrix adjoint operator \tilde{L} which when operating on the matrix of Green's

functions G_{ij} yields the following set of elements of the adjoint system $(\tilde{L}G)_{ij}$

$$(\tilde{L}G)_{1j} = -\frac{\partial G_{1j}}{\partial t} + \gamma \frac{\partial G_{2j}}{\partial t} - \frac{\partial^2 G_{1j}}{\partial y^2} \qquad (17)$$

$$(\tilde{L}G)_{2j} = \lambda \frac{\partial G_{1j}}{\partial t} - \frac{\partial G_{2j}}{\partial t} - \alpha \frac{\partial^2 G_{2j}}{\partial y^2}$$
(18)

$$(\tilde{L}G)_{3j} = -\frac{\partial G_{3j}}{\partial x} + Sh(G_{3j} - G_{1j}\Big|_{y=0})$$
(19)

$$(\tilde{L}G)_{4j} = -\frac{\partial G_{4j}}{\partial x} + \frac{Nu}{Le}(G_{4j} - \alpha Le G_{2j}\Big|_{y=0}).$$
(20)

The details of the construction are more fully given in [18]. The construction of the adjoint system for the case when Nu and Sh are infinite has been given in [17].

and the homogeneous boundary conditions

$$\left.\frac{\partial G_{1j}}{\partial y}\right|_{y=0} + Sh(G_{3j} - G_{1j}\Big|_{y=0}) = 0$$
(23)

$$\left. \frac{\partial G_{2j}}{\partial y} \right|_{y=0} + Nu \left(\frac{1}{\alpha Le} G_{4j} - G_{2j} \right|_{y=0} \right) = 0 \quad (24)$$

$$\left. \frac{\partial G_{ij}}{\partial y} \right|_{y=1} = 0, \, i = 1,2; \, j = 1,2,3,4.$$
 (25)

Initial and inlet conditions which the G_{ij} must satisfy are given by

$$G_{11} = G_{12} = G_{21} = G_{22} = 0 \text{ when } (\tau - t) = 0$$

and $(\xi, \eta) \neq (x, y)$ (26)

 $\begin{array}{l} G_{31} = G_{32} = G_{41} = G_{42} = 0 \text{ when } \xi - x = 0, \\ \eta = 0 \text{ and } \tau - t > 0 & (27) \\ G_{13} = G_{23} = G_{14} = G_{24} = 0 \text{ when } \xi - x = 0, \\ y = 0 \text{ and } \tau - t > 0 & (28) \\ G_{33} = G_{34} = G_{43} = G_{44} = 0 \text{ when } \xi - x = 0, \\ \tau - t > 0. & (29) \end{array}$

An integral representation of the vector of solution functions $U_j(\tau, \xi, \eta), j = 1, 2, 3, 4$, can now be written as

$$U_{j}(\tau,\xi,\eta) = \int_{0}^{\xi} \int_{0}^{1} \left\{ \left[G_{1j}(\tau,\xi,\eta;0,x,y) - \gamma G_{2j}(\tau,\xi,\eta;0,x,y) \right] U_{1}(0,x,y) + \left[G_{2j}(\tau,\xi,\eta;0,x,y) - \lambda G_{1j}(\tau,\xi,\eta;0,x,y) \right] U_{2}(0,x,y) \right\} dx dy + \int_{0}^{\tau} \left[G_{3j}(\tau,\xi,\eta;t,0) U_{3}(t,0) + G_{4j}(\tau,\xi,\eta;t,0) U_{4}(t,0) \right] dt + \int_{0}^{\xi} \int_{0}^{\xi} \left[G_{1j}(\tau,\xi,\eta;t,x,1) \frac{\partial U_{1}(t,x,1)}{\partial y} + \alpha G_{2j}(\tau,\xi,\eta;t,x,1) + \frac{\partial U_{2}(t,x,1)}{\partial y} \right] dx dt.$$
(30)

Using the Dirac delta function notation and summarizing the construction in [18], one obtains that the G_{ii} must satisfy

$$(\tilde{L}G)_{ij} = \delta_{ij}\delta(\tau - t)\,\delta(\xi - x)\,\delta(\eta - y),$$

 $i = 1,2; \quad j = 1,2,3,4$ (21)

$$(\tilde{L}G)_{ij} = \delta_{ij} \,\delta(\tau - t) \,\delta(\xi - x),,$$

 $i = 3,4; \quad j = 1,2,3,4$ (22)

For the non-homogeneous case, where

$$(LU)_i = F_i(t, x, y), i = 1, 2; (LU)_i = F_i(t, x),$$

 $i = 3, 4$ (31)

we add the following terms to the right hand side of equation (30)

$$\int_{0}^{\tau} \int_{0}^{\xi} \int_{0}^{1} \sum_{i=1}^{2} F_{i}(t, x, y) G_{ij}(\tau, \xi, \eta; t, x, y) dy dx dt + \int_{0}^{\tau} \int_{0}^{\xi} \sum_{i=3}^{4} F_{i}(t, x) G_{ij}(\tau, \xi, \eta; t, x) dx dt.$$
(32)

Physical interpretation

Each element G_{ij} of the Green's function matrix has an interesting physical interpretation. For example, $G_{11}(\tau, \xi, \eta; t_0, x_0, y_0)$ is the dimensionless concentration at time τ and the point (ξ, η) due to an instantaneous unit source of mass released at time t_0 at the point (x_0, y_0) . Similarly $G_{12}(\tau, \xi, \eta; t_0, x_0, y_0)$ is the dimensionless temperature at time τ and the point (ξ, η) due to an instantaneous unit source of mass released at time t_0 at the point (x_0, y_0) . In a like fashion we can give a physical interpretation for the remaining elements of the Green's function matrix.

Notice that the elements in the third and fourth rows (i = 3 or 4) of the Green's function matrix have no functional dependence upon y and that elements in the third and fourth columns (j = 3 or 4) have no functional dependence upon η .

INFINITE NUSSELT AND SHERWOOD NUMBERS

In some physical applications the resistance to mass and heat transfer between flowing fluid phase in the channel and the interface of the porous media is negligible. This will be the case for turbulent flow or for flow through systems where the tortuosity of the path of flow causes considerable mixing. It will also occur when the diffusivity in the matrix is much lower than in the channel, as in molecular sieves, or when the channel is very thin. By neglecting this resistance mathematical simplification is obtained.

If we allow the parameters Nu and Sh to approach infinity, the system of equations to be solved is (1), (2), (7) and (8) with boundary conditions (9) and (10). The remaining boundary, initial, and inlet conditions remain unchanged. The integral representation, equation (30) still holds; however, in the adjoint system of equations for the Green's functions equations (19), (20) are replaced by

$$(\mathcal{L}G)_{3j} = -\frac{\partial G_{3j}}{\partial x} - \frac{\partial G_{1j}}{\partial y}\Big|_{y=0}$$
(33)

$$(\tilde{L}G)_{4j} = -\frac{\partial G_{4j}}{\partial x} - \alpha \frac{\partial G_{2j}}{\partial y}\Big|_{y=0}$$
(34)

and boundary conditions given by equations (23) and (24) become

$$G_{3j} = G_{1j}|_{y=0} \tag{35}$$

$$G_{4j} = \alpha Le \; G_{2j} \big|_{y=0}. \tag{36}$$

Using (35) and (36) we can eliminate G_{3j} and G_{4j} from (33) and (34). From boundary conditions (9) and (10) we see that we need only to have a solution for $U_1(t, x, y)$ and $U_2(t, x, y)$. Therefore for the remainder of this section we shall restrict *j* to taking on only the values 1 and 2.

In other words we need only solve for the submatrix

$$\begin{bmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{bmatrix}$$

Anticipating in advance that τ and t and ξ and x will enter the Green's functions as $\tau - t$ and $\xi - x$, make the change of variables $t' = \tau - t$ and $x' = \xi - x$.

The adjoint system of equations and boundary conditions become

$$\frac{\partial G_{1j}}{\partial t'} - \gamma \frac{\partial G_{2j}}{\partial t'} - \frac{\partial^2 G_{1j}}{\partial y^2} = \delta_{1j} \,\delta(t') \,\delta(x') \,\delta(\eta - y)$$
(37)

$$-\lambda \frac{\partial G_{1j}}{\partial t'} + \frac{\partial G_{2j}}{\partial t'} - \alpha \frac{\partial^2 G_{2j}}{\partial y^2}$$
$$= \delta_{2j} \delta(t') \delta(x') \delta(\eta - y) \quad (38)$$

$$\frac{\partial G_{1j}}{\partial x}\bigg|_{y=0} - \frac{\partial G_{1j}}{\partial y}\bigg|_{y=0} = 0$$
 (39)

$$\left. \frac{\partial G_{2j}}{\partial x'} \right|_{y=0} - \frac{1}{Le} \frac{\partial G_{1j}}{\partial y} \right|_{y=0} = 0 \qquad (40)$$

$$G_{1j} = G_{2j} = 0$$
 when $t' = 0, x' > 0$ (41)

$$\left. \frac{\partial G_{1j}}{\partial y} \right|_{y=1} = \left. \frac{\partial G_{2j}}{\partial y} \right|_{y=1} = 0 .$$
 (42)

Equations (37) and (38) can be written in matrix form as:

$$\begin{bmatrix} 1 - \gamma \\ -\lambda & 1 \end{bmatrix} \begin{bmatrix} \frac{\partial G_{1j}}{\partial t} \\ \frac{\partial G_{2j}}{\partial t} \end{bmatrix} - \begin{bmatrix} 1 & 0 \\ 0 & \alpha \end{bmatrix} \begin{bmatrix} \frac{\partial^2 G_{1j}}{\partial y^2} \\ \frac{\partial^2 G_{2j}}{\partial y^2} \end{bmatrix}$$
$$= \delta(t) \,\delta(x) \,\delta(\eta - y) \begin{bmatrix} \delta_{1j} \\ \delta_{2j} \end{bmatrix}$$
(43)

where for convenience we have dropped the primes on t and x. Define the following matrices:

$$B = \begin{bmatrix} 1 & -\gamma \\ -\lambda & 1 \end{bmatrix}$$
(44)

$$G(t, x, y) = \begin{bmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{bmatrix} .$$
(45)

Multiplying equation (43) by B^{-1} gives the matrix equations:

$$\frac{\partial G}{\partial t} + A \frac{\partial^2 G}{\partial y^2} = H \tag{46}$$

where

$$A = \frac{1}{1 - \lambda \gamma} \begin{bmatrix} -1 & -\gamma \alpha \\ -\lambda & -\alpha \end{bmatrix}$$
(47)

$$H = \frac{\delta(t)\,\delta(x)\,\delta(\eta-y)}{1-\lambda\gamma} \begin{bmatrix} 1 & \gamma \\ \lambda & 1 \end{bmatrix} .$$
(48)

From their definitions

$$\lambda \gamma = \frac{1}{\left[1 + \frac{\varepsilon}{(1 - \varepsilon) K}\right] \left(1 + \frac{\rho_p C_p}{q K_t}\right)} \cdot (49)$$

From the second law of thermodynamics it can be shown that K and qK_t are positive quantities. Therefore, equation (49) shows that $0 < \lambda \gamma$ < 1 or equivalently $1 - \lambda \gamma > 0$. Thus the problem of division by zero is avoided in equations (47) and (48).

Let P be a non-singular matrix such that $PAP^{-1} = \Lambda$, where Λ is a diagonal matrix (for the present we are assuming that such a P exists). Premultiplying equation (46) by P and substituting $PA = \Lambda P$ we obtain:

$$P\frac{\partial G}{\partial t} + \Lambda P\frac{\partial^2 G}{\partial y^2} = PH$$
(50)

let

$$\Psi = PG. \tag{51}$$

Since the elements of P are constants they can be brought inside the differential operators $\partial/\partial t$ and $\partial^2/\partial y^2$ so that we obtain:

$$\frac{\partial \Psi}{\partial t} + \Lambda \frac{\partial^2 \Psi}{\partial y^2} = PH.$$
 (52)

The characteristic roots of $[-(1 - \lambda \gamma) A]$ are

$$r_1 = \frac{1}{2} \{ (1 + \alpha) + \sqrt{[(\alpha - 1)^2 + 4\alpha\lambda\gamma]} \}$$
 (53)

$$r_2 = \frac{1}{2} \left[(1 + \alpha) - \sqrt{[(\alpha - 1)^2 + 4\alpha\lambda\gamma]} \right].$$
 (54)

Following Henry [13] we could name the above roots a concentration root and a temperature root. When the coupling is weak so that λ and γ are small or α is extremely large one of the above roots approaches α , the coefficient of the Laplacian operator in the dimensionless temperature equation, and the other root approaches unity, the coefficient in the dimensionless concentration equation. However, as Henry said, ".... when coupling exists all roots are concerned with both diffusion processes to a greater or lesser extent."

The dimensionless groups α , and $\lambda \gamma$ are all positive numbers. Hence $(\alpha - 1)^2 + 4\alpha\lambda\gamma > 0$, and the characteristic roots of A are distinct. This is sufficient condition that a non-singular matrix P exist such that $PAP^{-1} = \Lambda$, a diagonal matrix. The matrices P, P^{-1} , and Λ are found to be:

$$P = \begin{bmatrix} -\lambda & 1 - r_1 \\ -\lambda & 1 - r_2 \end{bmatrix}$$
(55)

$$P^{-1} = \frac{-1}{\lambda(r_1 - r_2)} \begin{bmatrix} 1 - r_2 & -(1 - r_1) \\ \lambda & -\lambda \end{bmatrix}$$
(56)
$$A = \begin{bmatrix} \frac{-r_1}{1 - \lambda\gamma} & 0 \\ 0 & \frac{-r_2}{1 - \lambda\gamma} \end{bmatrix} .$$
(57)

Define

$$a_i = \frac{r_i}{1 - \lambda \gamma}, i = 1, 2.$$
 (58)

An alternate expression for r_2 is

$$r_{2} = \frac{1}{2} \{ (1 + \alpha) - \sqrt{[(\alpha + 1)^{2} - 4\alpha(1 - \lambda\gamma)]} \}$$
(59)

from which we see that r_2 is always positive. Therefore, the a_i defined in equation (58) are positive quantities. Using subscript notation we can now write equation (52) as

$$\frac{\partial \Psi_{ij}}{\partial t} - a_i \frac{\partial^2 \Psi_{ij}}{\partial y^2} = \delta(t) \,\delta(x) \,\delta(\eta - y) \,Q_{ij}, \, i, j = 1,2$$
(60)

where

$$Q = \frac{1}{1 - \lambda \gamma} \begin{bmatrix} -\lambda r_1 & 1 - \lambda \gamma - r_1 \\ -\lambda r_2 & 1 - \lambda \gamma - r_2 \end{bmatrix}$$
$$= \begin{bmatrix} -\lambda a_1 & 1 - a_1 \\ -\lambda a_2 & 1 - a_2 \end{bmatrix}. \quad (61)$$

Equations (39) and (40) can be rearranged into the following matrix equation

$$\frac{\partial G}{\partial y}\Big|_{y=0} = \begin{bmatrix} 1 & 0 \\ 0 & Le \end{bmatrix} \frac{\partial G}{\partial x}\Big|_{y=0} .$$
(62)

Using the substitution $G = P^{-1} \Psi$ we obtain

$$\left. \frac{\partial \Psi}{\partial y} \right|_{y=0} = R \left. \frac{\partial \Psi}{\partial x} \right|_{y=0}$$
(63)

where the matrix R is defined as

In subscript notation we have as the partial differential equations and boundary conditions that Ψ_{ii} must satisfy:

$$\frac{\partial \Psi_{ij}}{\partial t} - a_i \frac{\partial^2 \Psi_{ij}}{\partial y^2} = \delta(t) \,\delta(x) \,\delta(\eta - y) \,Q_{ij} \quad (65)$$

$$\frac{\partial \Psi_{ij}}{\partial y}\Big|_{y=0} - \sum_{k=1}^{\infty} R_{ik} \frac{\partial \Psi_{kj}}{\partial x}\Big|_{y=0} = 0 \quad (66)$$

$$\Psi_{ij} = 0 \text{ when } t = 0 \tag{67}$$

$$\left. \frac{\partial \boldsymbol{\Psi}_{ij}}{\partial y} \right|_{y=1} = 0. \tag{68}$$

We solve the above system by means of a double Laplace transform with respect to t and x. Inversion of the transform with respect to the transformed x-variable can be accomplished analytically. Inversion with respect to the transformed t variable, however, must be done by means of the inversion theorem and contour integration in the complex plane. The solution vector U is then obtained by substituting G and the appropriate initial, inlet and boundary conditions into equation (30) and performing the indicated integration. For constant initial and inlet conditions a somewhat simpler approach can be taken. Since the system of partial differential equations, equations (1)-(4), is linear we can choose the dimensionless temperature and concentration so that the initial conditions are zero. For zero flux at y = 1 we can write the solution for constant inlet conditions of U_3^0 and U_4^0 as

$$U_{f}(\tau,\xi,\eta) = U_{3}^{0} \int_{0}^{\tau} G_{3f}(\tau-t,\xi,\eta) dt + U_{4}^{0} \int_{0}^{\tau} G_{4f}(\tau-t,\xi,\eta) dt.$$
(69)

In the above the functional dependence on the four variables, τ , t, ξ and x has been indicated

$$R = P \begin{bmatrix} 1 & 0 \\ 0 & Le \end{bmatrix} P^{-1} = -\frac{1}{r_1 - r_2} \begin{bmatrix} -(1 - r_2) + Le(1 - r_1)(1 - r_1)(1 - Le) \\ (1 - r_2)(Le - 1) & (1 - r_1) - Le(1 - r_2) \end{bmatrix}.$$
 (64)

in terms of only two new variables, $\tau - t$ and $\xi - x$. Applying the convolution theorem, the Laplace transform U_j with respect to time is

$$\overline{U}_{j}(s, \xi, \eta) = U_{3}^{0} \frac{1}{s} \overline{G}_{3j}(s, \xi, \eta) + U_{4}^{0} \cdot \frac{1}{s} \overline{G}_{4j}(s, \xi, \eta)$$

$$= U_{3}^{0} \sum_{k=1}^{2} P_{1k}^{-1} \frac{1}{s} \overline{\Psi}_{kj}(s, \xi, 0; \eta)$$

$$+ U_{4}^{0} \alpha Le \sum_{k=1}^{2} P_{2k}^{-1} \frac{1}{s} \overline{\Psi}_{kj}(s, \xi, 0; \eta). \quad (70)$$

In the above, each Ψ_{ij} is considered as a four place function $\Psi_{ij}(\tau - t, \xi - x, y; \eta)$. Thus we see that we need only the Laplace inverse of $1/s \overline{\Psi}_{ij}(s, \xi, 0; \eta)$. It is this function which we actually invert by means of the inversion

φ

The symbol R_{ir}^{-1} denotes the inverse of the matrix R_{ir} .

In the above expression it should be noticed that the symbol *i* when used as a subscript is only an index; otherwise it denotes the imaginary unit $\sqrt{(-1)}$. The value of the integral in the above expression is given by the following expressions.

$$\lim_{\varepsilon \to 0} \frac{1}{\pi} \int_{\varepsilon}^{\infty} Re\left[e^{iyt} f_{ij}(iy)\right] dy$$
$$= \frac{2}{\pi} \int_{0}^{\infty} \frac{1}{u} \left[C_{Iij} \varphi_R\left(\frac{u}{\sqrt{(a_j)}}, \eta\right) + C_{Rij} \varphi_I\left(\frac{u}{\sqrt{(a_j)}}, \eta\right) \right] du \qquad (72)$$

$$_{R}(u,\eta) = \frac{\cosh\eta u \cos(2-\eta) u + \cos\eta u \cosh(2-\eta) u}{\cosh 2u + \cos 2u}$$
(73)

$$\varphi_{I}(u,\eta) = -\frac{\sinh \eta u \sin(2-\eta) u + \sin \eta u \sinh(2-\eta) u}{\cosh 2u + \cos 2u}$$
(74)

$$C_{Rij} = \sum_{k=1}^{2} e^{A_k} \left[Re \ m_{ijk} \cos \beta_k - Im \ m_{ijk} \sin \beta_k \right]$$
(75)

$$C_{Iij} = \sum_{k=1}^{2} e^{A_k} \left[Re \, m_{ijk} \sin \beta_k + Im \, m_{ijk} \cos \beta_k \right]$$
(76)

$$A_{k} = \frac{x}{2R} \left[-R_{11}B_{1}\left(\frac{u}{\sqrt{a_{2}}}\right) - R_{22}B_{1}\left(\frac{u}{\sqrt{a_{1}}}\right) \pm u(ReZ_{2} - ImZ_{2}) \right]$$
(77)

$$\beta_{k} = \frac{x}{2|R|} \left[-R_{11}B_{2}\left(\frac{u}{\sqrt{a_{2}}}\right) - R_{22}B_{2}\left(\frac{u}{\sqrt{a_{1}}}\right) \pm u(ReZ_{2} + ImZ_{2}) \right]$$
(78)

(71)

theorem. The details of this inversion are in [18]. We obtain the result as a real valued improper integral, where Re denotes the real part of a complex quantity.

 $+ \lim_{\varepsilon \to 0} \frac{1}{\pi} \int_{0}^{\infty} Re\left[e^{iyt} f_{ir}(iy)\right] dy \bigg\} \frac{Q_{rj}}{a_{r}}.$

 $L^{-1}\left\{\frac{1}{s}\overline{\Psi}_{ij}(s,x,0;\eta)\right\} = \sum^{2} \left\{\frac{1}{2}R_{ir}^{-1}\right\}$

In equations (77) and (78) the plus sign is chosen when k = 1, and the minus sign when k = 2. |R| is the determinant of the matrix R and is identically equal to the parameter *Le*.

$$B_1(u) = \frac{u(\sinh 2u - \sin 2u)}{\cosh 2u + \cos 2u}$$
(79)

$$B_2(u) = \frac{u(\sinh 2u + \sin 2u)}{\cosh 2u + \cos 2u} \tag{80}$$

 Z_2 is that branch of $\sqrt{(Z_1)}$ such that

$$-\frac{\pi}{2} < \arg Z_2 < \frac{\pi}{2}. \tag{81}$$

 Z_1 is a complex quantity whose real and imaginary parts are given by

$$ReZ_{1} = R_{11}^{2}(V_{2R}^{2} - V_{2I}^{2}) + R_{22}^{2}(V_{1R}^{2} - V_{1I}^{2}) + 2(R_{12}R_{21} - Le)(V_{1R}V_{2R} - V_{1I}V_{2I})$$
(82)
$$ImZ_{1} = 2R_{11}^{2}V_{2R}V_{2I} + 2R_{22}^{2}V_{1R}V_{1I} + 2(R_{12}R_{21} - Le)(V_{1R}V_{2I} + V_{1I}V_{2R})$$
(83)

$$V_{jR} = \frac{1}{\sqrt{(a_j)}} \frac{\sinh \frac{2u}{\sqrt{(a_j)}}}{\cosh \frac{2u}{\sqrt{(a_j)}} + \cos \frac{2u}{\sqrt{(a_j)}}}, j = 1, 2$$
(84)

$$V_{jI} = \frac{1}{\sqrt{(a_j)}} \frac{\sin \frac{2u}{\sqrt{(a_j)}}}{\cosh \frac{2u}{\sqrt{(a_j)}} + \cos \frac{2u}{\sqrt{(a_j)}}}, j = 1, 2$$
(85)

$$|Z_1| = \sqrt{[(Re Z_1)^2 + (Im Z_1)^2]}$$
 (86)

$$Re Z_2 = \sqrt{\left[\frac{1}{2}(Z_1 + Re Z_1)\right]}$$
 (87)

$$Im Z_2 = \pm \sqrt{\left[\frac{1}{2}(Z_1 - Re Z_1)\right]}.$$
 (88)

The sign in (88) is plus if $Im Z_1 \ge 0$ and minus if $Im Z_1 < 0$.

$$Re \ m_{111} = \frac{R_{22}}{2 |R|} + \frac{ReZ_2}{Z_2^2} \left[\left(1 - \frac{R_{11}R_{22}}{2 |R|} \right) V_{2R} - \frac{R_{22}^2}{2 |R|} V_{1R} \right] + \frac{ImZ_2}{Z_2^2} \left[\left(1 - \frac{R_{11}R_{22}}{2 |R|} \right) V_{2I} - \frac{R_{22}^2}{2 |R|} V_{1I} \right]$$
(89)

$$Re \ m_{112} = \frac{R_{22}}{|R|} - Re \ m_{111} \tag{90}$$

$$Rem_{121} = -\frac{R_{12}}{2|R|} + \frac{R_{12}}{2|R|Z_2^2} [ReZ_2(R_{11}V_{2R} + R_{22}V_{1R}) + ImZ_2(R_{11}V_{2I} + R_{22}V_{1I})]$$
(91)

$$Re m_{122} = -\frac{R_{12}}{|R|} - Re m_{121}$$
 (92)

$$Re \ m_{211} = \frac{R_{21}}{R_{12}}. \ Re \ m_{121} \tag{93}$$

$$Re \ m_{212} = \frac{R_{21}}{R_{12}} Re \ m_{122} \tag{94}$$

···· .

$$Re \ m_{221} = \frac{R_{11}}{2|R|} + \frac{ReZ_2}{Z_2^2} \left[\left(1 - \frac{R_{11}R_{22}}{2|R|} \right) V_{1R} - \frac{R_{11}^2}{2|R|} V_{2R} \right] + \frac{ImZ_2}{Z_2^2} \left[\left(1 - \frac{R_{11}R_{22}}{2|R|} \right) V_{1I} - \frac{R_{11}^2}{2|R|} V_{2I} \right]$$
(95)

$$Re m_{222} = \frac{R_{11}}{|R|} - Re m_{221}$$
(96)

$$Im \ m_{111} = -Im \ m_{112} = \frac{ReZ_2}{Z_2^2} \left[\left(1 - \frac{R_{11}R_{22}}{2|R|} \right) V_{2I} - \frac{R_{22}^2}{2|R|} V_{1I} \right] - \frac{ImZ_2}{Z_2^2} \left[\left(1 - \frac{R_{11}R_{22}}{2|R|} \right) V_{2R} - \frac{R_{22}^2}{2|R|} V_{1R} \right]$$
(97)

$$Im \ m_{121} = -Im \ m_{122} = \frac{R_{12}}{2|R|Z_2^2} \left[ReZ_2(R_{11}V_{2I} + R_{22}V_{1I}) - ImZ_2(R_{11}V_{2R} + R_{22}V_{1R}) \right]$$
(98)

$$Im \, m_{211} = \frac{R_{21}}{R_{12}} \, Im \, m_{121} \tag{99}$$

$$Im m_{212} = \frac{R_{21}}{R_{12}} Im m_{122} = -Im m_{211}$$
(100)

$$Im \, m_{221} = -Im \, m_{222} = \frac{ReZ_2}{Z_2^2} \left[\left(1 - \frac{R_{11}R_{22}}{2|R|} \right) V_{1I} - \frac{R_{11}^2}{2|R|} \, V_{21} \right] - \frac{ImZ_2}{Z_2^2} \left[\left(1 - \frac{R_{11}R_{22}}{2|R|} \right) V_{1R} - \frac{R_{11}^2}{2|R|} \, V_{2R} \right].$$
(101)

A computer program has been written to evaluate the four integrals defined by equations (72)-(101). The program, a listing of which is given in [18], also computes the value of the four functions $\int_{0}^{\tau} G_{ij}(\tau - t, \xi; \eta) dt$, i = 3, 4; j =1, 2 at the specified values of τ , ξ and η . The solution vector $U_{j}(\tau, \xi, \eta)$, j = 1, 2, is also computed for the specified constant inlet conditions U_{3}^{0} and U_{4}^{0} .

Verification of the solution

That the solution given by equations (69)-(101) satisfied the partial differential equations (1) and (2) and the boundary condition

$$\left.\frac{\partial U_j}{\partial y}\right|_{y=1} = 0$$

can readily be shown by substituting the solution into these equations. The inlet conditions can be shown to be satisfied identically by setting $\xi = \eta = 0$ and performing the indicated integration. Analytical verification of the equations

$$\frac{\partial U}{\partial x}\Big|_{y=0} = \begin{bmatrix} 1 & 0\\ 0 & \frac{1}{Le} \end{bmatrix} \frac{\partial U}{\partial y}\Big|_{y=0}$$
(102)

was not obtained because of the algebraic complexity of the resulting expressions. Numerical verification of (102) was obtained, however, by using the solution to calculate numerical values for the individual terms. Similarly, numerical verification of the zero initial conditions was obtained by setting $\tau = 0$ in the computer program input.

It should be noticed that if Le = 1, the matrix *R* reduces to the identity matrix, and equations (65) and (66) are uncoupled. Setting Le = 1yielded numerical results from the computer program which checked results obtained previously for the decoupled problem [18].

Therefore, in view of these numerical and analytical verifications, it is felt that the solution and computer program are correct.

Computer time required

Using an IBM 360/40 the time required to calculate results at each desired point (τ, ξ, η) averages about 6-7 s for longitudinal coordinate $\xi > 2$. For smaller values of ξ , convergence of the integrals in equation (72) is slower, requiring in some extreme cases as much as one min of computer execution time. Thus, even for the lengthy cases, it is felt that the solution presented here offers considerable computational advantages over the strictly finite difference approach, both in time required and in accuracy. Using the solution presented here, one is able to calculate results for those particular (τ, ξ, η) points desired rather than march out the entire solution up to the desired point as is necessary with the finite difference approach. This can result in considerable savings of computer time.

Application to drying

Using dimensions representative of actual drying equipment, breakthrough curves and transverse concentration and temperature profiles were calculated for the drying of moist air with silica gel. Saturated air at 25°C is assumed to enter 3 in. long cylindrical channels of 0.3 cm effective dia. at a bulk velocity of 1 ft/s. The internal walls of the channel are assumed to be coated with porous silica gel 0.05 cm thick.

From Lee and Cummings [21] we can approximate the silica gel-water equilibrium relationship by

$$\Gamma = \frac{0.02644\ CT}{P_s(T)} \tag{103}$$

where Γ is weight of sorbed water per weight of silica gel, C is moisture concentration in the gas phase in g/cm³, T is degrees Kelvin and $P_s(T)$ is the vapor pressure of water in atmospheres at temperature T. Inlet moisture concentration is calculated to be 0.230×10^{-4} g/cm³. We will assume that initial temperature is 50°C. As a point about which to linearize Γ we will choose $C = 0.115 \times 10^{-4}$ g/cm³ and $T = 38^{\circ}$ C.



FIG. 2. Sorption of H_2O on silica gel—concentration breakthrough curve, x = 9.25.

Figures 2 and 3 show the time response at the exit to a step change in inlet concentration. The solid lines refer to the case of a -25° C step change in inlet temperature; the dashed line is for zero change in inlet temperature.

The most interesting feature of the curves is that actually two breakthroughs in concentration and temperature occur. After the first breakthrough, the responses level off on a plateau which appears to correspond to a



FIG. 3. Sorption of H_2O on silica gel--temperature breakthrough curve, x = 9.25.

psuedo steady state condition. After remaining a while at this condition a second breakthrough occurs during which the responses move to their final values. The isothermal response, shown in Fig. 4, shows only the single breakthrough. The two breakthroughs are obviously due to the coupling between temperature and concentration. This phenomenon is better understood in the light of a thermodynamic analysis [18, 19]. In this analysis the resistances due to diffusion and heat conduction are neglected and only the equilibrium coefficients and convective transport terms are considered. This results in a hyperbolic system of two coupled first order partial differential equations whose solution has the form of two steps



FIG. 4. Isothermal concentration breakthrough curve at x = 9.25.

travelling at two distinct characteristic velocities. Resistances due to diffusion and heat conduction have the effect of speeding up the characteristic velocities and smoothing the steps into sigmoids. It should be added that the numerical results presented here differ little from a Nu and Sh number of 3, presented in [18] and [19].

Figure 5 presents transverse concentration and temperature profiles at the exit for two dimensionless times corresponding to 12.5 and 25 s.

In conclusion the authors would like to add that they recently learned that the phenomenon of two distinct breakthroughs, as predicted from the theoretical analysis presented here, has been observed experimentally in commercial type drying equipment [22, 23].

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FIG. 5. Sorption of H₂O on silica gel-transverse profiles.

REFERENCES

- J. B. ROSEN, Kinetics of a fixed bed system for solid diffusion into spherical particles, J. Chem. Phys. 20, 387-394 (1952).
- A. ANZELIUS, Ueber Erwaermung vermittals durchstroemender Medien, Z. Angew. Math. Mech. 6, 291 (1926).
- 3. T. E. W. SCHUMANN, Heat transfer: a liquid flowing through a porous prism, J. Franklin Inst. 208, 405 (1929).
- 4. F. W. LARSEN, Rapid calculation of temperature in a regenerative heat exchanger having arbitrary initial solid and entering fluid temperatures, *Int. J. Heat Mass Transfer* 10, 149–168 (1967).
- 5. M. JAKOB, *Heat Transfer*, Vol. 2, pp. 275–314. John Wiley, New York (1957).
- S. MASAMUNE and J. M. SMITH, Transient mass transfer in a fixed bed, *I/EC Fundamentals* 3, 179–181 (1964).
- S. MASAMUNE and J. M. SMITH, Adsorption rate studies: interaction of diffusion and surface processes, *A.I.Ch.E.JI* 11, 34-40 (1965).
- 8. M. WERNICK, Solution of fixed bed adsorption equations for general inlet and initial conditions by means

of Green's principle, I and II, *I/EC Research Results* Service MS 66-400-T and MS-401-T (1966).

- 9. P. M. MORSE and H. FESHBACH, Methods of Theoretical Physics, Vol. II. McGraw-Hill, New York (1953).
- 10. C. W. OSEEN, Neuere Methoden und Ergenbnisse in der Hydrodynamik. Akademische Verlagsgesellschaft, Leipzig (1927).
- C. E. BULLOCK, Dehumidification of moist air by adiabatic adsorption, Ph.D. Thesis, University of Minnesota, Minneapolis (1965).
- 12. CHANG WHAN CHI, Dynamics of fixed bed adsorbers, Ph.D. Thesis, Illinois Institute of Technology, Chicago (1968).
- P. S. H. HENRY, Diffusion in absorbing media, Proc. R. Soc. 171A, 215–41 (1939).
- 14. A. V. LUIKOV and Y. A. MIKHAILOV, *Theory of Energy* and Mass Transfer. Pergamon Press, New York (1965).
- P. NORDEN and H. G. DAVID, Coupled diffusion of moisture and heat in hygroscopic textile materials, *Int.* J. Heat Mass Transfer 10, 853-66 (1967).
- O. A. MEYER and T. W. WEBER, Nonisothermal adsorption in fixed beds, A.I.Ch.E.Jl 13, 457-65 (1967).
- 17. C. A. CHASE, DIMITRI GIDASPOW and R. E. PECK,

Diffusion of heat and mass in a porous medium with bulk flow: Part I. Solution by Green's functions. Part II. Application to fuel cells, *A.I.Ch.E. Symposium Series No. 92*, **65**, 91–109 (1969).

- C. A. CHASE, Unsteady coupled heat and mass transfer with bulk flow, Ph.D. Thesis, Illinois Institute of Technology, Chicago (1968).
- C. A. CHASE, DIMITRI GIDASPOW and R. E. PECK, Adiabatic adsorption in a regenerator, A.I.Ch.E. Symposium Series No. 96, 65 (1969). To be published.
- 20. C. A. CHASE, DIMITRI GIDASPOW and R. E. PECK, A regenerator Prediction of Nusselt numbers, *Int. J. Heat Mass Transfer* **12**, 727–736 (1969).
- H. LEE and W. P. CUMMINGS, A new design method for silica gel air dryers under nonisothermal conditions, *A.I.Ch.E. Preprint* 34E presented at 59th annual meeting, Detroit, December (1966).
- F. W. LEAVITT, Nonisothermal adsorption in large fixed beds, *Chem. Engng Prog.* 58, 54-59 (1962).
- 23. R. J. GETTY and W. P. ARMSTRONG, Drying air with activated alumina under adiabatic conditions, *Ind. Engng Chem.-Process Design & Dev.* 3, 60–65 (1964).

TRANSPORT DE CHALEUR ET DE MASSE TRANSITOIRE DANS UN REGENERATEUR ADIABATIQUE—REPRESENTATION PAR UNE MATRICE DE GREEN

Résumé—On propose un modèle mathématique décrivant le transport de chaleur et de masse transitoire à l'intérieur d'un milieu poreux avec un écoulement en bloc dans un conduit adjacent. Ce processus physique correspond à des échangeurs de masse du type régénérateur dans lesquels un soluté est enlevé d'une phase fluide par sorption sur la surface interne d'un matériau poreux.

On présente une formulation intégrale de la solution du modèle mathématique à l'aide de fonctions de Green. Une fois que les fonctions de Green sont déterminées, la solution du problème pour n'importe quelle condition arbitraire d'entrée, initiale et aux frontières est obtenue aisément par des intégrales d'évaluation faisant intervenir les fonctions de Green et les conditions connues. La solution du problème mathématique pour le cas dans lequel la production de chaleur et de masse a lieu à l'intérieur du matériau poreux 'peut aussi s'écrire immédiatement comme une intégrale faisant intervenir les fonctions de Green et les foncti de de

Dans le cas spécial où la résistance au transport de chaleur et de masse entre la phase s'écoulant dans le conduit et la surface extérieure du milieu poreux est négligeable, les fonctions de Green sont déterminées dans le domaine de Laplace de la variable temporelle. Des solutions exactes utilisant ces fonctions de Green sont obtenues pour des conditions initiales constantes et des conditions en échelon à l'entrée. Ces solutions permettent le calcul des profils de température et de concentration à l'intérieur du matériau poreux lui-même. De telles solutions sont sous la forme d'intégrales impropres, qui sont mieux évaluées à l'aide d'un calculateur numérique.

On a trouvé que les courbes de sortie pour l'échangeur de masse adiabatique présentent actuellement deux fronts à la différence du front unique présenté par l'échangeur de masse isotherme.

INSTATIONÄRER WÄRME- UND STOFFAUSTAUSCH IN EINEM ADIABATEN REGENERATOR

Zusammenfassung--Es wird ein mathematisches Modell zur Beschreibung der instationären wärme- und Stoffübertragung in einem porösen Medium mit Propfenströmung in einem anschliessenden Kanal vorgeführt. Dieser physikalische Prozess beschreibt einen Regnerativ-Stoffaustauscher bei dem eine Lösung aus der flüssigen Phase in die inneren Querschnitte des porösen Mediums wandert. Eine integrale Formulierung der Lösung des mathematischen Modells in Ausdrücken der Green'schen Funktion wird angegeben. Wenn die Green'schen Funktionen bestimmt sind, kann die Lösung des Problems für alle beliebigen Eintritts-, Anfangs- und Randbedingungen leicht erhalten werden durch Auflösung der Integrale unter Benutzung der Green'schen Funktion und der bekannten Bedingungen. Die Lösung des mathematischen Problems für den Fall der Wärme- und Stofferzeugung im porösen Material kann ebenfalls sofort ermittelt werden als Integral, das die Green'schen Funktionen und die bekannten Beziehungen für die Entstehung von Wärme und Stoff einschliesst.

Für den Sonderfall, vernachlässigbaren Widerstands beim Wärme- und Stoffaustausch zwischen strömendem Medium im Kanal und der Aussenfläche des porösen Mediums, sind die Green'schen Funktionen im Laplace'schen Gebiet durch die Zeitvariable bestimmt. Mit diesen Green'schen Funktionen erhält man exakte Lösungen für konstante Anfangsbedingungen und stufenweise Änderungen der Zugaben am Eintritt. Diese Lösungen erlauben die Festlegung von Temperatur- und Konzentrationsprofilen im porösen Material. Solche vollständigen Lösungen für einfache Probleme sind vorläufig in der Literatur nicht bekannt. Diese Lösungen sind angegeben in Form uneigentlicher Integrale, welche sich am besten auf einem Digitalrechner auswerten lassen.

Es wurde festgestellt, dass die Durchbruchs-Kurven für den adiabaten Stoffaustauscher zwei Durchbrüche zeigen im Gegensatz zu nur einem Durchbruch beim isothermen Stoffaustauscher.

НЕСТАЦИОНАРНЫИ ТЕПЛО-И МАССООБМЕН В АДИАБАТИЧЕСКОМ РЕГЕНЕРАТОРЕ.

МАТРИЧНЫЕ ПРЕДСТАВЛЕНИЯ ФУНКЦИЙ ГРИНА

Аннотация—Предлагается математическая модель для описания нестационарного тепло-и массообмена в пористой среде с течением в прилежащем канале. Этот физический процесс характерен для массообменников регенеративного типа, в которых растворенное вещество абсорбируется из жидкой фазы на внутреннюю поверхность пористого материала.

Интегральная формулировка решения математической модели дается в функциях Грина. После того, как определены функции Грина, легко получается решение задачи для любых произвольных входных, начальных и граничных условий путем оценки интегралов, включающих функции Грина и известные условия. Решение математической задачи для случая выделения тепла в пористом материале может быть также непосредственно записано в виде интеграла, включающего функции Грина и известные функции, описывающие выделение тепла и массы.

Для частного случая пренебрежимо малого сопротивления тепло-и массообмену между текучей фазой в канале и наружной поверхностью пористой среды функции Грина определены в лапласовой области переменной по времени. При использовании этих функций Грина получены точные решения для постоянных начальных условий и ступенчатого изменения на входе. Эти решения позволяют рассчитать профили температуры и концентрации в самом пористом материале. Такие решения аналогичных задач до сих пор не были опубликованы в литературе. Эти решения получены в виде несобственных интегралов, которые удобнее всего рассчитать на цифровой вычислительной машине. Установлено, что кривые абсорбционного цикла для адиабатического массообменника имеют две критических точки в противоположность изотермическомумассообменники сообмением солость изотермическому-

массообменнику, характеризующемуся одной критической точкой.

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