

SHORTER COMMUNICATIONS

A SPECIAL CASE OF DIFFUSION WITH MOVING BOUNDARY CONSIDERED AS A PROPAGATING WAVE

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NOMENCLATURE

- a , position of boundary;
- a_0 , position of boundary at time $t = 0$;
- A , area;
- c , concentration of diffusant;
- c_a , concentration of diffusant at boundary;
- c_{a0} , initial concentration in the first, limited medium;
- c_0 , initial concentration;
- D , diffusivity of diffusant;
- M , total amount of diffusant;
- q , penetration distance of diffusant;
- Q , total amount of diffusant normalized by area;
- t , time;
- v , moving velocity of boundary;
- x , distance.

and

$$c(x, t) = \frac{3.5Q}{3.5a + q} \left[1 - \frac{x - a(t)}{q} \right]^{2.5} \quad \text{for } x > a(t). \quad (5)$$

As may be verified by a simple calculation, equations (4) and (5) are solutions of the homogeneous linear partial differential equation

$$\frac{\partial c}{\partial t} + v \frac{\partial c}{\partial x} + \frac{3.5vc}{3.5a + q} = 0. \quad (6)$$

It is known [2, 3] that the most simple linear differential equation to represent a wave has the form

$$\frac{\partial c}{\partial t} + v \frac{\partial c}{\partial x} = 0, \quad v = \text{const.} \quad (7)$$

For the initial condition $c(x, t) = c_0(x)$, this equation gives the solution

$$c(x, t) = c_0(x - vt). \quad (8)$$

This solution represents a wave travelling with constant profile and with the velocity v in the positive x -direction. Figure 1 suggests that a similar equation could fit the experimental results, after additionally making allowance, of course, for the increasing dilution. The introduction of the attenuation term $3.5vc/(3.5a + q)$ into equation (7) is made to conform with this requirement and permits a complete description of the concentration profiles to be made. The term $3.5vc/(3.5a + q)$ also makes sense physically: the attenuation is greater the faster the wave moves, and the greater the concentration is; on the other hand, it decreases as the boundary advances and with increasing penetration distance.

It is essential that the concentration profile is not restricted to that given by equation (5), but beyond the boundary it can also be described by other functions, such as the steady-state solutions of the partial differential equations of diffusion.

The present paper makes no statement on processes before

A PREVIOUS paper [1] we considered the diffusion of a solute from a first, limited medium into a second, unlimited medium. The total amount of diffusant remains constant and is initially restricted to the first medium. The boundary between both media migrates with constant velocity in the direction of the second medium. Within the first medium, the diffusant remains equipartite throughout the equilibration process, i.e.

$$c(x, t) = c_a(t) \quad \text{for } 0 \leq x < a(t). \quad (1)$$

At steady-state within the second medium, the following concentration profile applies (Fig. 1):

$$c(t) = c_a(t) \left[1 - \frac{x - a(t)}{q} \right]^{2.5} \quad \text{for } x > a(t) \quad (2)$$

then

$$a(t) = a_0 + vt$$

and

$$v = \frac{da}{dt}$$

The total amount of diffusant, normalized by area, is given by

$$Q = \frac{M}{A} = c_a(t) \left[a(t) + \frac{q}{3.5} \right]. \quad (3)$$

Figure 1 presents the corresponding relations: with increasing time, the concentration profile advances in the positive x -direction, whilst, because of the concomitant increase in dilution, the concentration is fading more and more; at the next time, however, the decreasing concentration distribution to the right of the boundary retains its shape.

These circumstances and the postulate of equation (3), requiring the total amount of diffusant to be constant, are taken into account by the equations

$$c(x, t) = \frac{3.5Q}{3.5a + q} \quad \text{for } 0 \leq x < a(t) \quad (4)$$

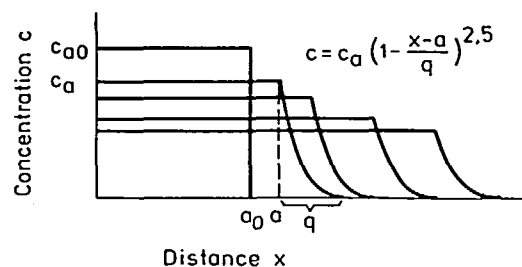


FIG. 1. Concentration distribution with moving boundary.

the attainment of steady state (during "swinging in"). According to Peterlin [4], the time necessary approximately amounts to $4D/v^2$.

Comparison of experimental concentration profiles (ref. [1], Fig. 2) with values calculated from equations (4) and (5) shows relatively good conformity, at which, as in ref. [1], the time to reach the equilibrium has to be considered, as well as the fact that the precision of measurement diminishes with decreasing impulse count.

The occurrence of diffusion waves is of special interest for the co-operation of chemical reactions and diffusion. The present paper tries to extend the analogy between wave propagation and diffusion processes to the particular experimental case of diffusion with a moving boundary.

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SOME COMMENTS ON BECK'S SOLUTION OF THE INVERSE PROBLEM OF HEAT CONDUCTION THROUGH THE USE OF DUHAMEL'S THEOREM

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NOMENCLATURE

a ,	radius of cylinder or sphere;
erfc ,	complementary error function;
E ,	depth of thermocouple below heated surface;
F_r ,	least-square function;
Fo ,	Fourier number, $\alpha t/L^2$ or $\alpha t/a^2$;
J_0/J_1 ,	Bessel function of the first kind of order zero and unity, respectively;
k ,	thermal conductivity;
L ,	thickness of slab;
q_i ,	heat flux at time $t_i = i\Delta t$;
\bar{q}_i ,	heat flux at time t_i determined by exactly matching the thermocouple data over r future times;
\bar{q}_{i+1} ,	constant value of heat over the time interval t_i to t_{i+r} that minimizes the least-square error function F_r ;
r ,	radial coordinate, also the number of future temperatures used in inverse solution;
T ,	temperature;
T_E^i ,	computed temperature at time t_i and depth E below the heated surface;
\bar{T}_E^i ,	value of T_E^i corresponding to \bar{q}_i ;
T_0 ,	initial temperature;
t ,	time;
w^i ,	heat-flux weighting factor for a thermocouple at depth E , see equation (20);
x ,	coordinate;
Y^i ,	experimental thermocouple data at time $t_i = i\Delta t$.

Greek symbols

ΔFo ,	differential Fourier number, $\alpha\Delta t/L^2$ or $\alpha\Delta t/a^2$;
Δq_i ,	step change in heat flux, equation (2);
Δt ,	time increment;
$\Delta\phi^i$,	$\phi^i - \phi^{i-1}$, $\phi^0 = 0$;
α ,	thermal diffusivity;
λ ,	dummy time variable;
v ,	eigenvalue in equations (4)-(6);
ϕ ,	temperature response of a body initially at zero temperature and subjected to a unit step in heat flux, also termed sensitivity coefficient;
ϕ_E^i ,	value of ϕ at depth E and time t_j ;
ψ ,	function representing decay of temperature profile if future heat-flux values are zero, see discussion following equation (9);

w_E^i , temperature weighting factor for a thermocouple at depth E ; see equation (16).

INTRODUCTION

THE INVERSE problem of heat conduction is the determination of surface temperature and/or heat flux from an interior measurement of temperature. For those problems to which Duhamel's Theorem applies, Beck [1] introduced a technique for using measurements of future temperatures that allows for smaller computational steps than those allowed in the earlier technique of Stolz [2]. This note presents equations that permit an alternative physical interpretation of the process of using future temperature information, and gives additional insight into inverse heat conduction problems.

ANALYSIS

Starting with the 1-dim. form of Duhamel's Theorem, for a time-varying heat flux,

$$T(x, t) = T_0 + \int_0^t \phi(x, t-\lambda) \frac{dq}{d\lambda} d\lambda + \sum_{i=0}^n \phi(x, t-\lambda_i) \Delta q_i \quad (1)$$

where

$$\Delta q_i = q_i - q_{i-1}, \quad q_0 \equiv 0$$

and where $\phi(x, t)$ is the temperature response of a body initially at zero temperature and subjected to a unit step in heat flux. The integral term in equation (1) allows for continuous variation of heat flux with time; the summation term accounts for discrete steps in heat flux. Many analytical solutions for bodies exposed to a step in heat flux are available in the literature; four solutions for common 1-dim. geometries are presented below.

Semi-infinite solid, flux at $x = 0$

$$\phi(x, t) = \frac{2}{k} \left[\left(\frac{\alpha t}{\pi} \right)^{1/2} e^{-x^2/4\alpha t} - \frac{x}{2} \operatorname{erfc} \frac{x}{2(\alpha t)^{1/2}} \right]. \quad (3)$$