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A Note on Setting Up the Diffusion Equation

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A Note on Setting Up the Diffusion Equation

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A NOTE ON SETTING UP THE DIFFUSION EQUATION

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ABSTRACT

Traditionally, the transient heat conduction equation and other diffusion-type equations have invariably been expressed in the form of a partial differential equation. In this paper we address the question, how will the governing equation look if, instead of invoking infinitesimal calculus, one writes down the mass balance or energy balance statements directly for a discrete elemental volume of arbitrary shape? This inquiry leads us to taking a careful look at the physical, empirical basis of concepts such as conductivity and capacitance on the on hand and their idealization in the context of a continuum as embodied in the transient diffusion equation. Many intriguing questions arise about such issues as, how one may arrive at a unique initial condition based on data at a finite number of points, how fluxes may be evaluated correctly when potentials are continuously changing with time at either end of a flow tube and how one may define capacitance for a poorly stirred calorimeter. The discussions presented suggest that it is worth our while to explore the foundations of the transient diffusion equation which we use widely to understand an enormous variety of physical systems.

Leave the beaten tracks occasionally and dive into the woods. You will be certain to find something you have never seen before.

Alexander Graham Bell

INTRODUCTION

The transient heat conduction (diffusion) equation is widely used in the earth sciences to quantitatively understand a variety of processes including heat transfer, fluid flow in subsurface systems, chemical diffusion (in liquids and solids) and the flow of electricity. Following Fourier, who in the early 19th century wrote down the governing equation of heat conduction in solids for the first time, the diffusion equation is invariably written as a partial differential equation. This equation, which physically represents the conservation of mass or energy over an infinitesimally small elemental volume, is derived by starting with a volume element of finite size, writing the terms for fluxes and accumulation, normalizing the accumulation by the bulk volume of the element and collapsing the element in the limit to a point. In this work we address the question: suppose we do not wish to give ourselves a differential equation. Suppose we wish to look at the balance equation directly at the level of a discrete elemental volume of a finite size. What would such an inquiry lead to? As will be seen, the inquiry raises some intriguing issues concerning the foundations of the transient diffusion equation.

TRADITIONAL PRACTICE

It has become almost second nature for us to derive the partial differential equation for diffusion-type problems by starting with a regularly-shaped box or a cylindrical annulus whose six faces are orthogonal to the axes of the chosen coordinate system (Figure 1). Following this, we write expressions for mass balance as a prelude to setting up the differential equation. The task of establishing mass balance itself does not demand the use of any of these regular-shaped elements. Traditionally we chose these types of elements of a regular shape for a specific reason. These elements have a simple well-defined relation between surface area and volume. Thus, when surface area is divided by volume, we are left with a length term in the denominator. In turn, upon letting this length tend in the limit to zero, we obtain the second derivative in space. Indeed, normalization by bulk volume is merely an artifact devised to create the second derivative in space. Despite these artifacts, we recognize that the resulting partial differential equation has served us extraordinarily well

for nearly two hundred years. The main reason for its success is that it transformed a problem of integration (summation of fluxes) over discrete domains into an equivalent mathematical problem involving spatial and temporal gradients which could be handled in terms of continuous functions having algebraic forms. The resulting closed-form solutions, series solutions or integrals have provided us enormous insights into diffusion-type processes.

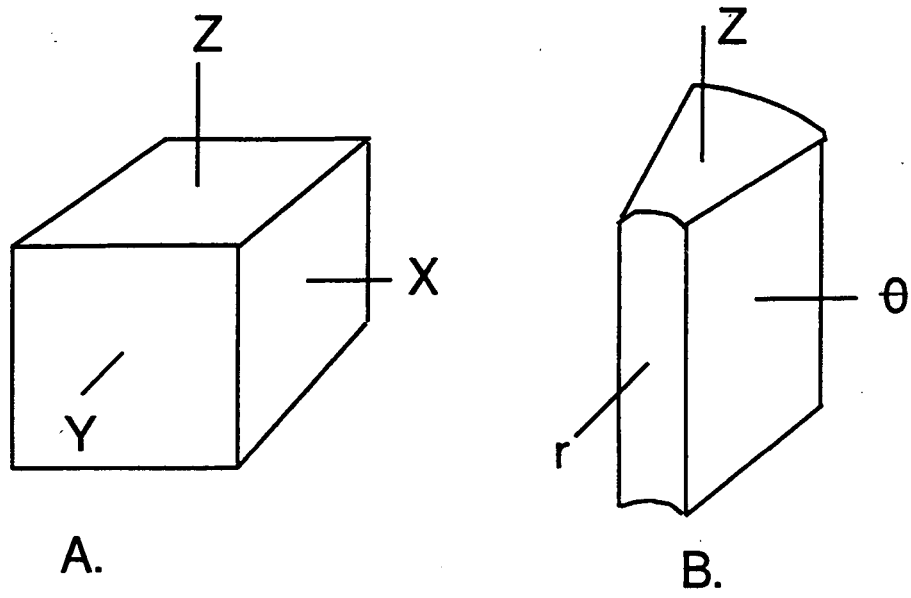

Figure 1: Discrete volume elements used to derive the transient diffusion equation. (A) Cartesian coordinates, and (B) Cylindrical coordinates

AN ALTERNATE PERSPECTIVE

Let us now consider the notion of mass balance from a different perspective which does not commit itself to deriving the differential equation. Instead, one simply takes a careful look at the

process of mass balance over a discrete elemental volume and addresses its implication to spatial and temporal distribution of potentials.

INITIAL CONDITIONS

Consider an arbitrary elemental volume as shown in Figure 2A. This elemental volume exists within a larger transient flow domain of complicated geometric shape. Let us assume for simplicity that the entire domain is occupied by a single homogeneous isotropic material. At the time instant t_0 portrayed in the figure, there exist surfaces of equal potential as shown schematically. Perpendicular to the isopotential surfaces are flow lines. In practice, these isopotential surfaces and flow lines are to be inferred from observations of potential at discrete locations or points.

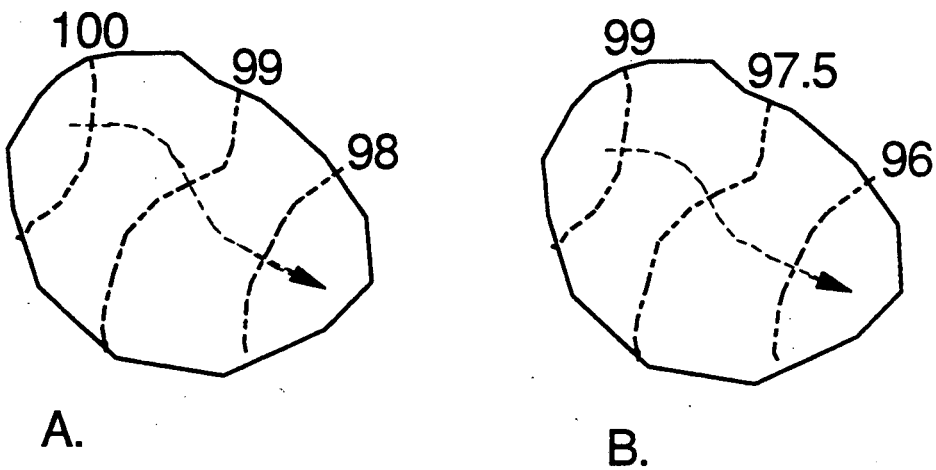

Figure 2: An arbitrary elemental volume bounded by the solid line and its isopotential surfaces. Arrows represent flow lines: (A) at time $t = t_0$, and (B) at time $t = t_0 + \Delta t$

We now start with a set of points at which potentials are known at a certain instant in time. The isopotential surfaces shown in Figure 2 imply that the flow domain constitutes a continuum in which potential is a continuous function in space and in time. An important question now arises: how does one deduce a continuous surface from the values of potential known at a finite number of discrete points? Clearly an infinite number of continuous surfaces can fit the values at a finite number of points. Consequently, if we desire to have a unique surface fitting the potentials at these points, we have to impose appropriate constraints on the nature of the surface to be so chosen. For example, we may stipulate that the surface satisfies the constraints of steady state diffusive transport over the flow domain. We can show that under steady state diffusive transport, the required surface fitting the point values of potential must satisfy two conditions as detailed below.

Condition 1: In Figure 3A is shown a set of hypothetical points in a steady state system occupied by a homogeneous isotropic material within a domain of arbitrary geometry at a given instant in time. The potentials at these points are assumed to be known. Because of the arbitrary geometry of the flow domain, the local flow pattern is characterized by converging and diverging flow paths. The isopotential contours in the figure have been drawn by using some arbitrarily chosen interpolation function (e.g. linear interpolation between adjacent points). The flow lines are oriented perpendicular to the isopotential contours. In Figure 3A we see two flow tubes, the steady flux through one of these is Q_A. Based on empirical observations, the relation between Q_A and the isopotential surfaces can be expressed in the mathematical form of Ohm's Law,

$$Q_A = \frac{\Delta \Phi}{R} \quad , \tag{1}$$

where R is resistance to flow and $\Delta\Phi$ is the drop in potential. In this context, if we consider two segments of the flow tube in the figure having flux Q_A, their resistances R_1 and R_2 must be equal because the potential drop $\Delta\Phi$ is the same over both these segments. A corollary to equation 1 is that potential drop $\Delta\Phi$ is directly proportional to resistance along the flow tube. Therefore, (1) can also be used to interpolate between two isopotential surfaces and find the position of intermediate values of isopotentials on the basis of the proportional relation between $\Delta\Phi$ and R.

Condition 2: In Figure 3B is shown the same situation as in Figure 3A but with a difference. In this figure, the position of the intermediate isopotential surface with contour value 85 has been found by interpolation within the two adjacent flow tubes. These surfaces meet at P, a point on the interface between the adjoining flow tubes. If contour lines have no error in them, then the isopotential surface 85 must be continuous at P.

Thus the continuous surface fitting the point values must satisfy two criteria. First, within a given flow tube, resistances over equal drops in potential must be equal. Secondly, isopotential surfaces must be continuous at interface between adjacent flow tubes. These two criteria together constitute sufficient conditions to fit a unique surface through the points at which potentials are known at a given instant in time.

Going back to Figure 2A now, it is in this sense that we assume that the isopotential lines and the flow line have been drawn. Nevertheless, the element in Figure 2 represents the state at a given instant in time in *a transient* system. Yet, the contours have been drawn using *steady state* assumptions. We thus have a difficulty; a system cannot simultaneously exist under steady conditions and under transient conditions. How may we overcome this contradiction? To overcome this difficulty, should we dispense with the notion of isopotential surfaces and flow lines in a transient system? The answer has to be "no" because the use of an equation of motion (Darcy's Law, Fourier's Law) is essential to the formulation of the equation governing the transient flow process. In turn, these empirically defined equations are defined only in terms of steady-state experiments and the notion of a flow tube is intrinsic to these equations. Thus, the notion of a flow tube is essential to the formulation of the transient equation. Under the circumstances, perhaps the only way to get around this difficulty of the flow domain existing simultaneously under steady and transient flow conditions is simply to postulate that the transient system evolves in time in such a way that at any every instant in time the potentials satisfy spatial equilibrium in the sense of the empirical, steady-state equation of motion.

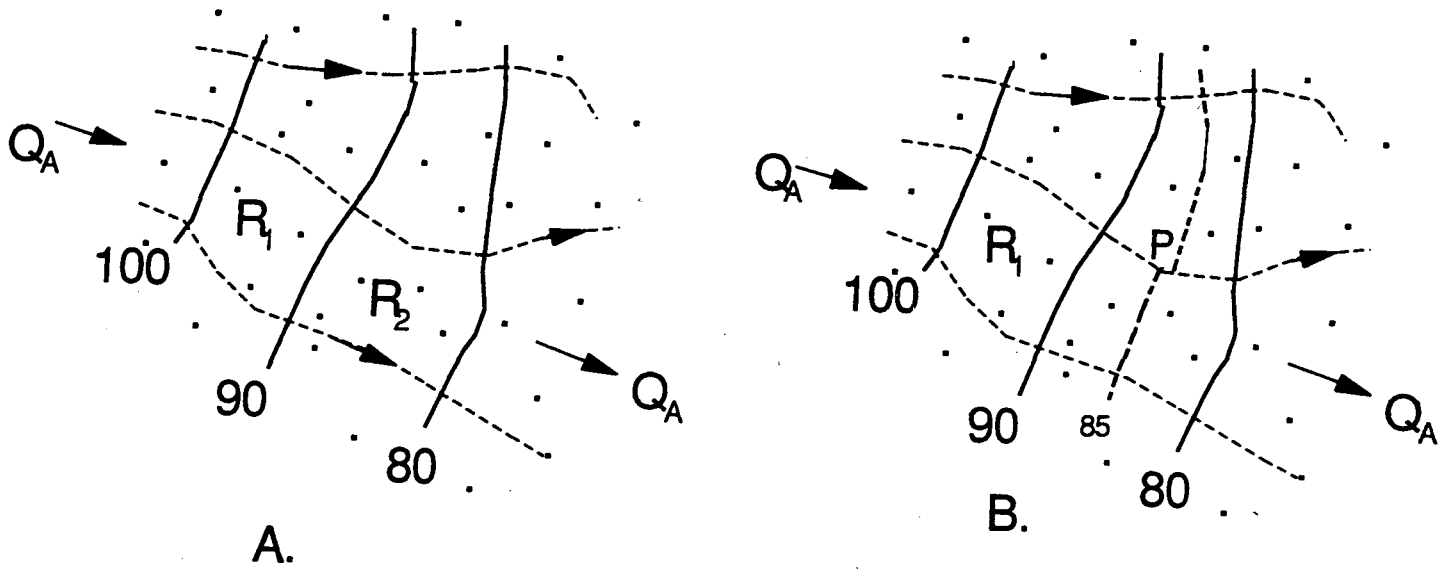

Figure 3: Fitting a continuous surface over a set of point values; constraining conditions (A) resistances along flow tube, (B) continuity of isopotential surfaces

CHANGE OF STATE AND CAPACITANCE

Having considered the "state" of the elemental volume at a given instant in time, let us consider how the system may change its state with time. Let $t = t_0$ be the instant at which the state of the element is as shown in Figure 2A. Let Δt represent an interval of time such that $t = t_0 + \Delta t$. If the flow domain is existing under transient conditions, the isopotential contours would have shifted in position over Δt. In the most general case, both the shapes and the magnitudes of the isopotential surfaces would have changed. Consequently, the change in potential $\Delta\Phi$ over the time interval would

be different at different locations within the elemental volume. Our problem is, given the state of the element at $t = t_0$, find the positions and magnitudes of the isopotential contours at $t = t_0 + \Delta t$.

Now suppose we are some how able to get the net accumulation over the element in Figure 2 during the interval Δt. Then, in order to convert this accumulation into a change in potential $\Delta\Phi$, we need the capacitance of the element. Here, capacitance of a finite volume or mass of material is defined as accumulation per unit change in potential. This notion of capacitance comes from the study of heat and dates back to Lavoisier and Laplace in 1783. Fundamentally, the notion of capacitance is associated with a calorimeter. In order that the heat capacitance of the mass of material be uniquely defined, the mass of material in question must change from one *thermostatic state* to another *thermostatic state*. This is the reason why a calorimeter has to be well mixed when one wishes to determine heat capacity of a liquid such as water. When the change in temperature is the same everywhere in the mass of material, heat accumulation can be divided by a uniquely prescribed ΔT (that is, change in temperature) and heat capacity is determined unambiguously.

With this background, consider the element in Figure 2A and Figure 2B. Neither its initial state at $t = t_0$ nor its final state at $t = t_0 + \Delta t$ are motionless static states. Nor are the changes in potential $\Delta\Phi$ the same everywhere within the element. Because of this, $\Delta\Phi$ cannot be uniquely specified over the element. Therefore, even though accumulation is known precisely, we cannot uniquely stipulate a capacitance for the elemental volume because the denominator $\Delta\Phi$ is undefined. In essence, the element is much like a poorly stirred calorimeter. Conversely, if we know the accumulation exactly and wish to determine change in potential within the element, we will have to use different values of capacitance for different locations within the element. That is, the capacitance of an elemental volume in a transient system has to be viewed as a function of the nature of the material *as well as the particular location* within the element where $\Delta\Phi$ is desired to be determined.

In summary, we see that the experimentally inspired notion of capacitance is associated with a system which is considered to jump from one static state to another static state. Yet, we desire to use this concept of capacitance under transient situations in which static equilibrium does not exist. To overcome this dilemma, we may give an ad hoc status to parameter capacitance when dealing with transient systems. Consequently, in a transient system, capacitance has to be defined as a

function of the material constituting an elemental volume *as well as the location* at which change in potential is to be evaluated.

THE TRANSIENT EQUATION

We now proceed to combine the postulate concerning the equation of motion and the ad hoc extension of the notion of capacitance to assemble a governing equation for an elemental volume of finite size existing under transient conditions. Our logic is to first use the equation of motion to evaluate the accumulation over the elemental volume during Δt and use the suitably-defined capacitance of the element as a means of converting the accumulation into a change in potential at a specified location.

First, we devote attention to evaluating the fluxes that enter and leave the elemental volume. Traditionally, we are accustomed to using a flux law in a form that involves gradient of potential. That is,

$$Q_x = -K \frac{d\Phi}{dx} A , \tag{2}$$

where Q_x is the flux in the direction x along which the gradient of potential is evaluated, K is conductivity and A is area of cross section. However, this form is not convenient for us to use in the case of an elemental volume such as the one in Figure 2 because we have chosen not to make use of infinitesimal calculus. It is more advantageous for us to use the equation of motion in the form of Ohm's Law (1). Note that the empirical basis for the equation of motion is a flow tube bounded at the inlet and at the outlet by surfaces of equal potential. The material within the tube itself is assumed to be homogeneous in our present discussions. Although it is customary to do these experiments on a tube of uniform cross sectional area, we may reasonably extend the concept to non-uniform flow tubes for which the form of Ohm's Law applies. The denominator in Ohm's Law is the Resistance,

which includes both the material property (e.g. hydraulic conductivity) as well as the geometry of the flow tube. For a flow tube of nonuniform cross section, the resistance may be expressed as,

$$R = \int_{x_{in}}^{x_{out}} \frac{dy}{K\,A(y)} , \tag{3}$$

where A(y) expresses the variation of A as a function of position along a suitable flow path chosen as a curvilinear x axis.

The question now is, how may we apply the equation of motion in this form to a volume element of finite size?

A Logical Elemental Volume

In order that we may implement the equation of motion to be compatible with the empirical nature of the equation of motion, let us abandon a volume element of arbitrary shape as in Figure 2 and define a volume element j in the context of a flow tube as shown in Figure 4.

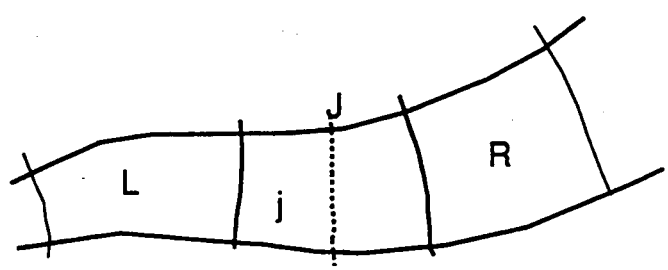

Figure 4: Three neighboring elemental volumes along a flow tube. j is the volume element of interest. L and R denote neighbors to the left and the right. J is a conveniently chosen isopotential surface whose magnitude will change with time.

We now write the mass balance equation for the middle element j in Figure 4. For simplicity, assume that over the time interval of interest to us, the position and shape of the flow lines remain unchanged. This is possible when we deal with a flow system of known symmetry (e.g. cylindrical or spherical) or in a transient system in which flow geometry changes very slowly in comparison to the time interval of interest. Although the shapes of the isopotential surface are fixed, their magnitudes will change in time. Within this element we have chosen the isopotential line denoted J for purposes of computing the change in potential. The change in potential $\Delta\Phi$ will be the same at any point along this surface. We now wish to write an expression for the change in potential along the chosen isopotential contour J. In order to do this we need to define a capacitance for the volume element j in such a way that when the accumulation over the element is divided by the said capacitance we will get the change in potential at any point on the chosen isopotential surface J. Thus,

$$C_j = \zeta V c \quad , \tag{4}$$

where C_j is the operational capacitance of element j, ζ is a positive coefficient , V is the bulk volume of the element and c is the specific capacitance (capacitance per unit volume). We need not dwell here on how ζ may be determined but simply stipulate that it can be chosen on the basis of appropriate physical reasoning.

Given these assumptions, the flux into j from the elements on either side can be summed up to yield the accumulation over an interval of time Δt by,

$$\text{Accumulation} = \Delta t \left[\sum_{k=L}^{k=R} \frac{1}{R_{kj}} \left(<\Phi_k> - <\Phi_j> \right) \right] \quad , \tag{5}$$

where $<\Phi_k>$ and $<\Phi_j>$ are potentials at k and j averaged over the time interval Δt and R_{kj} is the resistance of the flow tube segment bounded by the isopotential surfaces I and J.

We need to pause here and consider how the time-averaged values of potential may be evaluated rationally so that the fluxes and the accumulation implied in (5) are accurate. For illustration consider the flow tube segment between the element i, located to the left of j and j. This segment is shown in Figure 5. Normally, one would calculate the flux through this segment of the flow tube by assuming that flow is steady state and that the potentials Φ_i and Φ_j at the inlet and the outlet of this segment are independent of time. However, under transient conditions, both Φ_i and Φ_j vary continuously with time. How may one apply the equation of motion to a flow tube the potentials at the end of which change in time?

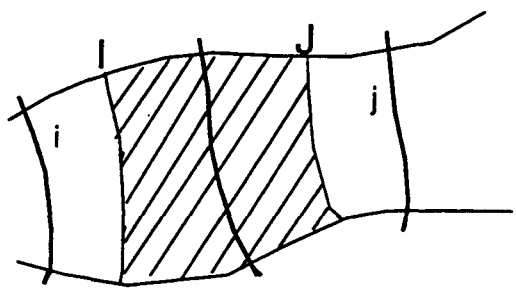

Figure 5: Flow tube between the isopotential surfaces I of element i and J of element j. The flow tube is shown by hatching

To understand this, consider the simple case of a flow tube initially under steady conditions of flow. At time t = 0, the potential at the inlet end is suddenly raised to a higher level and maintained constant. The potential at the other end continues to remain unchanged. Clearly, the flow tube will experience transient flow and the fluxes at the inlet and outlet will be unequal. With time, the flux at inlet will gradually decrease and the flux at outlet will gradually increase. After significant elapse of time, the flow tube will attain a new steady state. Upon attaining steady state, the inlet flux will match the outlet flux. This pattern of time-dependent flux change is illustrated in Figure 6. Note in Figure 6 that the outlet end will register an increase in flux only after a finite time interval needed for the perturbation in potential at the upstream end to travel to the downstream end. The total quantity of flow, $Q\Delta t$ entering the flow tube segment over the time interval will be equal to the area under the curve, shown by hatching. Effectively then, before steady conditions of flow are established, the actual quantity of flow over Δt will be different from what one might calculate by simply dividing the difference in potential by the resistance. In view of this, it is clear that the time-averaged values $<\Phi_k>$ and $<\Phi_j>$ should be so determined that due consideration is given to deviations from steady state assumptions. This discussion intrigues us about letting time tend in the limit to zero in deriving the transient equation because as Δt becomes small, the flow is prevented from attaining steady state.

In view of (5), we may write down an expression for the new potential along the isopotential surface J of element j at time $t = t_0 + \Delta t$ by,

$$\Phi_j(t_0+\Delta t) = \Phi_j(t_0) + \frac{\Delta t}{C_j}\left[\sum_{k=L}^{k=R} \frac{1}{R_{kj}}(<\Phi_k> - <\Phi_j>)\right] . \tag{6}$$

Equation 6 is essentially the governing equation for the discrete elemental volume j within a flow tube. This equation is valid for a volume element that is part of a curvilinear flow tube. In principle, one could directly program this equation into a computer algorithm towards solving problems. Should one so desire, one could invoke infinitesimal calculus and derive a partial differential equation for one dimensional flow in a flow tube with variable cross section as was shown by Fick (A. Fick, On Liquid Diffusion, Phil. Mag, 10, 30-39,1855),

$$\frac{\partial c^2}{\partial x^2} + \frac{1}{A}\frac{dA}{dx}\frac{\partial c}{\partial x} = \frac{\partial c}{\partial t} . \tag{7}$$

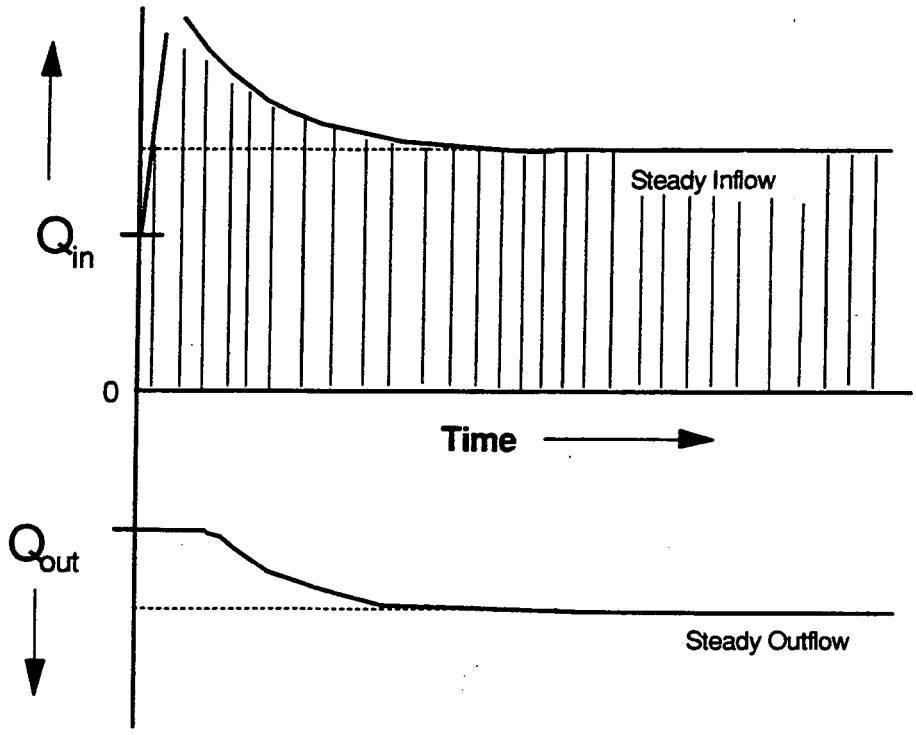

Figure 6: Time-dependent variation of fluxes at inlet and outlet of a flow tube subjected to a step-wise increase in inlet potential

The governing integral equation (6) pertains to a single flow tube. One way to extend this equation to general three dimensions is to consider the three dimensional system to be collection of flow tubes. One would write an equation such as (6) for each of the flow tubes. Having done this, one could impose suitable constraints of continuity of potential at interfaces between adjoining flow tubes. Note that this statement inherently treats the multidimensional problem in terms of a collection of parallel processes.

DISCUSSION

The derivations presented above have focused attention on a discrete elemental volume, unfettered by an ulterior desire to use a differential equation. The basic notions of resistance, capacitance and conservation relate to finite volumes of material. Although these three notions are physically meaningless at a point which intrinsically has no dimensions, the pioneers of mathematical physics of two centuries ago invented the artifact of the differential equation pertaining to a point because functional analysis provided a way of solving problems which were unsolvable otherwise. Without the contrived differential equation, there was no conceivable way of solving practical problems which needed to be solved to understand phenomena of nature. The availability of the tool dictated how the problem will be posed.

Two hundred years after Fourier, we now have a radically different tool available to us for solving mathematical problems. This tool is the computer. The computer simultaneously provides us the ability to store, retrieve and manipulate information pertaining to very complex mathematical objects and, in addition, solve a large number of algebraic equations intrinsically interwoven with the complex geometric objects. This new tool provides us a motivation to depart from the well-beaten track shown us by Fourier and explore a new track which perhaps is naturally suited to exploit the power of the digital computer as a means of solving problems of interest to us.

The differential equation is intimately tied up with vectors and hence is associated with specific coordinate systems, preferably rectilinear. However, using the differential equation with curvilinear coordinate systems can be cumbersome, even with the aid of tensors. As we have seen, the alternate development explored above is quite convenient to use in systems characterized by curvilinear coordinates, especially with the availability of the computer and the remarkable graphic tools that are available with the computer.

Aside from this possibility of using the computer for problem solving, the thoughts presented above are of interest in other ways. As we have seen, our foundations for describing the transient process lie on two equilibrium concepts; the equation of motion which assumes that potentials have achieved spatial equilibrium and the notion of capacitance which assumes that the potential is always in equilibrium with its appropriate extensive attribute (the equation of state). However, a system

cannot simultaneously be transient and at equilibrium. There is thus something fundamentally intriguing about the way we are using our empirical experience of steady state systems to quantify the behavior of dynamic systems.

The fact that solutions to differential equations have reasonably imitated the behavior of transient systems (e.g. transient heat conduction in a rod or cylinder) may be taken to suggest that our foundations are perfectly sound. This success of the differential equation may be taken to assert that in the limit of vanishing volume, one can assume simultaneous existence of steady and non-steady states within a system. The logical strength of this assertion deserves careful inquiry. As long as the volume does not vanish, the elemental volume in the continuum will contain infinitely many points and one has to reconcile the simultaneity of steady and non-steady states. On the other hand, if the elemental volume vanishes to a single point, notions of resistance, capacitance and potential conservation are invalid. Nor does a point have any symmetry.

Be that as it may, it is clear that whenever we are confronted with problems of sufficient complexity which require us to integrate the differential over discrete domains, one has to address the issues discussed above and lay down suitable postulates to enable logically sound numerical integration. Clearly, without properly defining what the integral is, one cannot reliably integrate a differential equation over discrete elemental volumes.

In closing, the purpose of this note is not to criticize the differential equation. Conceived by some of the most distinguished minds of the 18th and 19th centuries, modern science owes much of its success to the differential equation. Yet, we do recognize that some limitations are inherent to the methodology of the differential equation. It is in the best tradition of science to explore if we can find other methodologies which can help us look farther. It is in this spirit that this note has looked at the diffusion-type process directly in the context of a discrete domain of the continuum. It appears that the foundations of our traditional methodology may not be as strong as we might have thought.

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