LBNL-41235
UC-403
Preprint

ERNEST ORLANDO LAWRENCE
BERKELEY NATIONAL LABORATORY

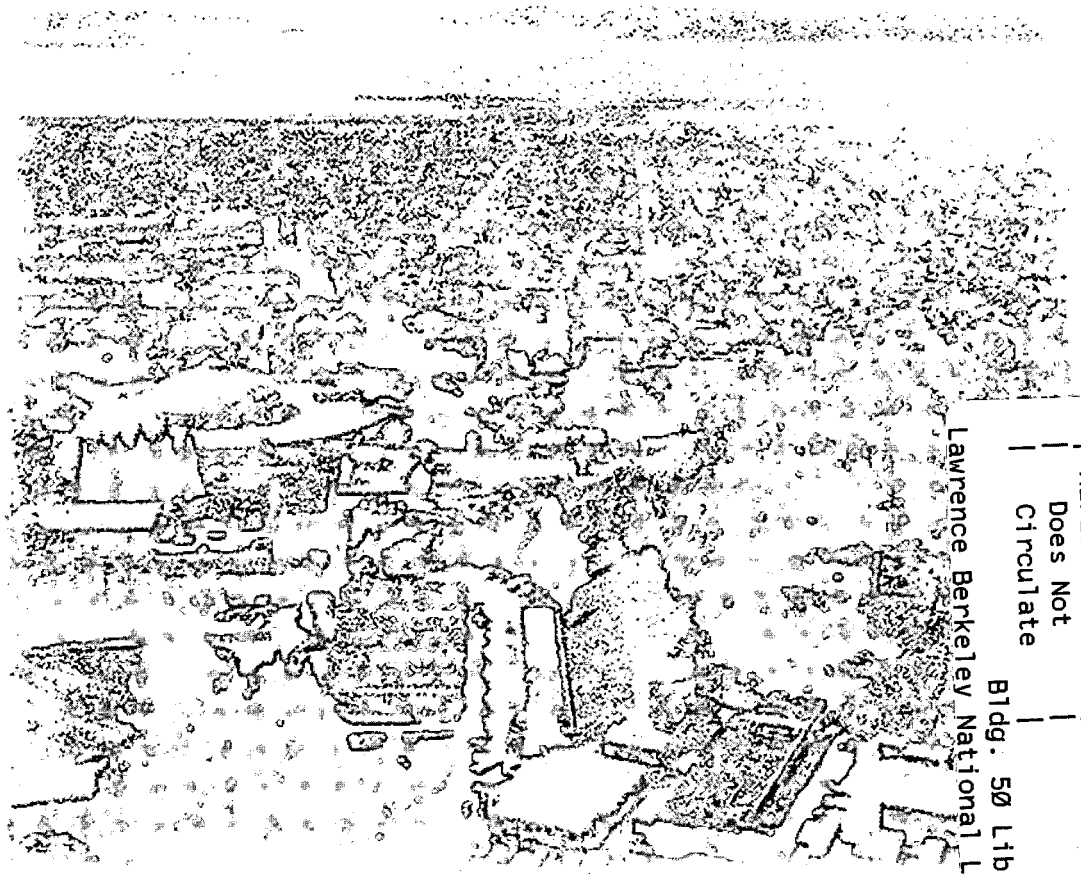
Basic Postulates of Groundwater Occurrence and Movement

T.N. Narasimhan

Earth Sciences Division

January 1998

Submitted to
Water Resources Research



REFERENCE COPY
Does Not
Circulate
Bldg. 50 Library - Ref.
Lawrence Berkeley National Laboratory
Copy 1
LBNL-41235

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

LBNL-41235
UC-403

Basic Postulates of Groundwater Occurrence and Movement

T.N. Narasimhan

Department of Materials Science and Mineral Engineering
and
Department of Environmental Science, Policy and Management
University of California, Berkeley

and

Earth Sciences Division
Ernest Orlando Lawrence Berkeley National Laboratory
University of California
Berkeley, California 94720

January 1998

This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

BASIC POSTULATES OF GROUNDWATER OCCURRENCE AND MOVEMENT

T.N. Narasimhan
Department of Materials Science and Mineral Engineering
Department of Environmental Science, Policy and Management
Earth Sciences Division, Ernest Orlando Lawrence Berkeley National Laboratory
University of California at Berkeley
467 Evans Hall, University of California at Berkeley, Berkeley, Ca 94720-1760

"May the well-disposed reader receive the performance with the same love for the object as that with which it is sent forth"

G.S. Ohm, Berlin, 1827.

ABSTRACT

For nearly two centuries, the partial differential equation of heat conduction has constituted the foundation for analyzing many physical systems, including those involving the flow of water in geologic media. Even as the differential equation continues to be a powerful tool for mathematical analysis in the earth sciences, it is useful to look at the groundwater flow process from other independent perspectives. The physical basis of the partial differential equation is the postulate of mass conservation. Alternatively, it is possible to understand groundwater movement in terms of energy and work because mechanical work has to be done in moving water against the resistance to flow offered by the solid material and to store water by opening up pore spaces. To this end, the behaviors of steady-state and transient groundwater systems are sought to be understood in terms of postulates concerning the state of a groundwater system, its tendency to optimally organize itself in response to impelling forces and its ability to store and release energy. This description of groundwater occurrence and flow, it is shown, is equivalent to the variational statement of the Laplace equation for the steady-state case and is similar to Gurtin's (1964) variational principle for the transient case. The approach followed here has logical similarities with Hamilton's principle for dynamical systems. Though the variational statement of the transient groundwater flow process is appealing in that it provides a rationale for deriving the parabolic equation, intriguing questions arise when one attempts to understand the physical significance of the variational statement. This work is motivated in part by a desire to develop a better understanding of the groundwater flow process from an intuitive base pertaining to discrete systems . Also, as we show an increasing preference to numerically solve groundwater flow problems on the basis of integro-differential equations, it is likely that the work presented here may contribute to improving such integral solution techniques.

INTRODUCTION

In 1807 Fourier formally stated the transient process of heat conduction in solids in the form of a partial differential equation and showed a way of solving the equation in terms of his newly discovered Fourier series. Since then, Fourier's differential equation has formed the mathematical foundation for analyzing a wide array of problems in mathematical physics, including groundwater flow. Even as we continue to use the differential equation to great advantage, it is useful to look at the groundwater flow process from alternate perspectives so as to independently assert the veracity of the classical differential equation and perhaps, to develop new insights.

The motivation for this work is two-fold. The first is one of curiosity. The simple experiment of Darcy and the infinitesimal calculus have led to such complex mathematical superstructures concerning flow and transport of fluids in porous media that one some times wishes to have an independent way of evaluating the worth of these superstructures in providing answers for scientific questions. Second, numerical methods used for solving dynamic groundwater flow problems are moving away from differential equations to integro-differential equations and integral equations. The domains of the integrals involved are discrete in space and in time. As one attempts to integrate the differential, one is confronted with issues of weighting functions and averaging rules. It stands to reason that such functions and averages should properly stem from physical postulates which govern the dynamical system. Thus, this work is also motivated in part by a desire to identify a comprehensible basis that is independent of the differential equation for formulating numerical models of groundwater flow and transport.

This work is restricted to isothermal groundwater flow systems in which compressible water moves through a deformable medium under conditions of laminar flow.

OCCURRENCE OF GROUNDWATER

WATER AS A HOST FOR MECHANICAL ENERGY

In its natural state, groundwater stores mechanical energy. The energy so stored comprises two components: one arises from its location in the earth's gravity field and the other arises from its ability to change geometry (that is, its ability to deform) in response to forces acting on it. The "pressure" of water is a manifestation arising from the interrelations between the geometry of a water packet and the forces that act on it.

POSTULATE 1: Equation of State for water

Given sufficient time, the volume (geometry) of a packet of water will attain a unique equilibrium with its pressure. The relationship between pressure and volume is an "equation of state". Volume and pressure are understood to be "state variables".

POROUS MEDIUM AS A HOST FOR WATER AND ENERGY

In groundwater systems water resides in porous media, which too, by virtue of their tendency to deform and to interact with fluids, have the ability to store mechanical energy. Geologic porous media deform in response to a combination of "stresses" which act externally on their skeleton and the pressure of water which exists internally within the pore spaces. In the present work we make the tacit assumption that external stresses remain unchanged at all times. Thus, the porous medium too is characterized by two state variables, namely, geometry and fluid pressure. The mass of water contained in a chunk of geologic material is equal to the product of its pore volume, its saturation and the mass density of water. In a geologic medium, water saturation is governed by water pressure in its manifestation as capillary pressure. Thus the mass of water contained in a chunk of geologic material is a function of water pressure.

Just as water, the porous medium too hosts energy, stemming from its ability change its geometry in response to pressure and its ability store energy at fluid-fluid interfaces. Therefore, the total energy stored in a geologic material by virtue of an increase in water pressure is a sum of the energy stored in water and that stored in the porous medium.

POSTULATE 2: Equation of State for the geologic medium containing water

Given sufficient time, a geologic material will attain a unique equilibrium between the mass of water contained in it and the water pressure existing inside it. Mass of water and water pressure constitute state variables for the water-containing geologic material. Here "water pressure" is understood to be macroscopic and measurable using instruments of finite size.

Two implications of this postulate are worth noting.

1. If either of the state variable changes, the other will change as prescribed by the equation of state.
2. It is assumed that sufficient time has been available for pressure and geometry to attain equilibrium. In other words, equation of state has an appropriate macroscopic time scale associated with it. If sufficient time has not been available for such an equilibration, then, geometry and pressure are said to be "kinetically" related.

MOTION OF GROUNDWATER

CAUSE OF MOTION

As described by Hubbert (1940) in his classic work, groundwater moves in response to impelling forces which act on it. Groundwater flow is "laminar" and the direction of movement is the same as that of the impelling force. The impelling force acts in the direction of decreasing concentration of energy in groundwater. The term "energy potential" is used when this concentration is expressed as mechanical energy per unit mass of water [L^2/T^2]. The impelling force is maximum in the direction of maximum descent of the energy potential.

A groundwater system comprises a spatial region enclosed within well-defined boundaries. The interior of the system comprises porous geologic materials permitting storage and flow of water, while the boundary experiences forces external to the system which cause groundwater to move within the system. Subject to the overall direction of movement dictated by the impelling forces acting on its external boundaries, the groundwater system responds by generating forces of reaction within the system. The forces of reaction are governed by a combination of the rate of mass flow (mass flux of water) occurring through the system as well as the ability of the geologic materials to offer mechanical resistance to the flow. Here, mass flux is defined as mass of water per unit time (dimensions, M/T)

Empirical justification for our notions of fluid motion and energy motion stem from the seminal contributions of Ohm (1827) and Darcy (1856) who investigated the steady movement of energy and water in well-defined flow tubes. Therefore, it is useful to think of laminar water motion in terms of macroscopic flow tubes of finite dimensions. A flow tube has an inlet and an outlet. It comprises a collection of non-intersecting flow lines which commence at the inlet where the potential is high and end at the outlet where the potential is low.

The effort involved in moving water through a flow tube is directly related to the magnitudes of the impelling force and the reactionary force. Whereas the impelling force is proportional to the potential drop, the reaction force is proportional to the mass flux. Thus, the potential drop is the "cause" and the mass flux is the "effect". The product of mass flux and potential at the inlet represents the rate at which energy is brought into the flow tube[1]. So also, the product of mass flux and potential at the exit represents the energy that taken out of the flow tube. Under steady-state conditions, the product of mass flux and the difference in potential between inlet and outlet denotes

---

[1] Here we neglect kinetic energy because groundwater velocities are known to be very small. Furthermore, as pointed out by Hubbert (1940), kinetic energy needs to be neglected if microscopic flow and macroscopic flow are to be kinematically similar, an assumption necessary to derive Darcy's Law

the rate at which energy is expended as work in moving water through the flow tube.

POSTULATE 3: Self-organization Tendency

A steady-state groundwater system is one in which the fluid potentials and the amounts of mass and energy stored remain unchanged in time. In such a system, the maximum and minimum potentials occur on the boundaries and the distribution of potentials on the boundaries define a set of inlets and outlets for water to enter or leave the system. Constrained by these inlets and outlets, the interior of the system will organize itself into a collection of flow tubes in such a manner that the rate at which work is done in moving water through the system is an extremum.

The above postulate implies that for prescribed impelling forces on the boundary, the system will maximize the throughput of water. Equivalently, for achieving a given throughput of water, the system will minimize the impelling forces.

HYDRAULIC RESISTANCE

Empirically (Ohm, 1827; Darcy, 1856) it was found that the laminar flux of water through a flow tube is directly proportional to the potential drop over the tube and the reciprocal of the constant of proportionality is the "hydraulic resistance" of the flow tube. Hydraulic resistance has the following properties: (a) it is additive along the flow path, (b) it increases with increasing flow length and, (c) it decreases with increasing area of cross section perpendicular to the flow path.

Thus, if the area of cross section over a small distance Δx of the flow tube is $A(x)$ and if r is the resistivity (dimensions, L^3 / [MT]) of the geologic material occupying the segment, then the hydraulic resistance (dimension, L^2/[MT]) of the segment is given by,

(1) $$R = \frac{r\,\Delta x}{A(x)} .$$

Given this, the additive property of hydraulic resistance enables us to write the hydraulic resistance of a flow tube in the form of a definite integral evaluated along a properly chosen flow path extending from the inlet to the outlet. Thus, if we choose the flow path as a general curvilinear x-axis, then,

(2) $$R = \int_{x_{inlet}}^{x_{outlet}} \frac{r\,dx}{A(x)} .$$

In view of these, we may express the mass flux of water through a flow tube i in the form of Ohm's Law,

(3)
$$Q_i = \frac{\Delta\Phi_i}{R_i} .$$

Behavior of a Steady-state Flow System

The self-organization tendency (Postulate 3) merits attention. Consider a steady-state groundwater flow system of arbitrary shape with potentials prescribed on several segments of the boundary. An example is shown in Figure 1 in which the flow region is subject to prescribed boundary potentials on five segments. Given sufficient time, the system can organize itself into an infinite number flow configurations; four of these are schematically shown in Figures 2a through 2d. In Figure 2a water enters the flow region through one inlet and leaves the flow region at four outlets. In Figure 2d, on the contrary, water enters the flow region across four different boundary segments and exits at one outlet. The particular flow geometry preferred by the system will be dictated by the self-organization postulate. Note, in figures 2a through 2d, that the flow system comprises three or four subsystems, each being a large flow tube of arbitrary shape. Recall that the rate of work done in a flow tube is equal to the product of the mass flux through the tube and the potential drop over the tube. Therefore, the self organization postulate requires that,

(4)
$$\Omega^* = \sum_i Q_i \Delta\Phi_i = \frac{(\Delta\Phi_i)^2}{R_i}, \quad i = \mathrm{I, II, III, IV}$$

be a maximum, given that the potential, Φ, has been prescribed on the boundary. Note that the magnitude of hydraulic resistance depends on the geometry of a flow tube as well as the physical nature of the materials occupying the flow tube. Thus, given a certain material distribution within the flow region, the system has the freedom to adjust the geometry of the flow tubes in such a way that the self-organization postulate is satisfied. It follows therefore that the particular flow geometry preferred by the system (figures 2a through 2d) will depend on the spatial distribution of materials of varying hydraulic resistivity (heterogeneity) occupying the flow region. In heterogeneous media, flow lines will refract at the interface between materials of contrasting hydraulic resistivity according to a law of tangents (Hubbert, 1940).

It is worth drawing attention here to an analogy with Joule's Law, which expresses the equivalence between electric current flowing through a resistive circuit and mechanical work expended as heat. Thus, (Maxwell, 1888),

(5) Heat generated measured in dynamical units =

Square of current X Resistance X Time.

Now, in (4) if we consider a single flow tube and recognize that $Q = \Delta\Phi/R$, we see that the work done during a time interval is,

(6)
$$\text{Work Done} = Q\Delta\Phi t = Q\frac{\Delta\Phi}{R}Rt = Q^2Rt \ .$$

Thus, the expression for work used in the present work for groundwater current is exactly analogous to that used for electric current in Joules's Law.

Relation to Variational Statement

The self-organization postulate discussed above in terms of a discrete set of flow tubes can be seen to become a variational principle for steady-state groundwater flow, if one invokes infinitesimal calculus and expresses the extremum condition in terms of an integral, rather than a discrete sum.

Let the flow region be discretized into i = 1,2,3,4..... I flow tubes. Let the potential drop over each flow be discretized into j = 1,2,3,4 ..... J intervals. Then the rate at which work is done over the jth potential drop of the ith flow tube may be written as,

(7)
$$\Omega_{ij} = \frac{(\Delta\Phi_{ij})^2}{R_{ij}} \ ,$$

where $\Delta\Phi_{ij}$ is the drop in potential and R_{ij} is the hydraulic resistance of segment ij. We may now proceed to sum this quantity over the entire flow region in order to derive the variational principle for steady-state groundwater flow. Thus,

(8)
$$\Omega^* = \sum_i \sum_j \frac{(\Delta\Phi_{ij})^2}{R_{ij}} .$$

With a few algebraic manipulations and invocation of infinitesimals, we now proceed to obtain an integral representation of Ω^*. Noting that hydraulic resistance, by definition, is $\Delta x/[r\ A(x)]$, we may rewrite Ω^* ,

(9)
$$\Omega^* = \sum_i \sum_j \frac{A_{ij}(\Delta\Phi_{ij})^2}{r\,\Delta x} .$$

Multiplying numerator and denominator by Δx and recognizing that $A\,\Delta x = \Delta V$, where V is volume, we get,

(10)
$$\Omega^* = \sum_i \sum_j \frac{(\Delta\Phi_{ij})^2\,\Delta V}{r\,(\Delta x)^2} .$$

For denoting the hydraulic resistive property of the material we now choose to use the parameter k^*, hydraulic permeability (dimension, MT / L^3), which, by definition, is the reciprocal of hydraulic resistivity, r. That is, $k^* = 1/r$. Then,

(11)
$$\Omega^* = \sum_i \sum_j \frac{k^*(\Delta\Phi_{ij})^2\,\Delta V}{(\Delta x)^2} .$$

Finally, if we let I and J tend to ∞ and Δx tend in the limit to 0, the discrete sum represented by Ω^*

becomes an integral,

$$\Omega = \int_V k^* (\nabla\Phi)^2 \, dV \quad . \tag{12}$$

Sometimes referred to as Euler's integral, this equation is used as the variational principle for the Laplace equation. That is, upon minimization, this integral leads to the Laplace equation as shown in Appendix 1.

Discussion

Since the integral has been derived purely from consideration of forces and resistances, it appears that Ω^* and Ω must be valid for saturated groundwater motion as well as for unsaturated groundwater flow. There exists a caveat, however. No groundwater system can instantaneously adjust itself to imposed changes on boundary forces. The system will require a finite amount of time to organize itself in order to be in equilibrium with the changed conditions. During the time the system takes to adjust itself, other physical processes such as change in storage (dictated by hydraulic capacitance), kinetic effects, hysteresis and so on may come into play. Assuming that such time-related effects do not exist, the self-organization postulate and the related variational principle are valid for heterogeneous groundwater systems in which hydraulic conductivity may be either dependent or independent of the energy potential Φ.

The partial differential equation of steady-state groundwater flow is known as the Laplace equation or an elliptic equation. This equation in distinguished from the Poisson equation which allows for the presence of source/sink terms in the elliptic equation. In groundwater systems, wells or boreholes are often treated as sources or sinks of vanishingly small radii for mathematical convenience. However, realistically speaking, wells and boreholes possess finite radii. Therefore, it is logical and appropriate to treat the inner surfaces of wells and boreholes as boundary surface rather than as abstract objects such as sources. Thus, the discussions presented above include physical situations covered by the Laplace equation as well as the Poisson equation.

Variational calculus is an important part of mathematical physics which seeks to provide basic insights into the behavior of physical systems. The variational perspective which developed below appears to have been motivated by a perception that the Laplace equation must be a derivative of a more primitive integral statement. In other words, one starts with the premise that a primitive integral Ω exists, which, when minimized or maximized appropriately, will yield the Laplace equation. A mathematical "search" for such a primitive integral appears to have led to the Euler's integral given

above. In the present work, we have approached the same issue from a different view point, based on an a priori enunciation of postulates concerning expected system behavior.

THE TRANSIENT FLOW PROCESS

At the outset it appears logical that the postulates presented above must be extendable, in a straight forward way, to transient flow of groundwater. However, a physically comprehensible variational statement of the transient groundwater flow process has as yet to be formulated. Purely from a mathematical point of view, Gurtin (1964) proposed a variational principle for the linear diffusion equation. Gurtin's variational principle, which involves convolution integrals, has been used by some as a basis for formulating numerical methods for solving the transient groundwater flow process. The physical import of Gurtin's variational principle is not clearly understood.

We now proceed to extend the set of postulates to include the transient groundwater flow process. We begin by identifying the physical attributes of the transient flow system.

ATTRIBUTES OF A TRANSIENT GROUNDWATER SYSTEM

1. In a transient groundwater system, mechanical energy is brought in across inlet segments and taken out across outlet segments of the system-boundary
2. Part of the energy that is brought into the system is expended in doing work to overcome resistive forces in order to move water and part of the energy is stored within the flow region through change in energy potential. The storage of energy is a reversible process. However, energy expended in moving water is an irreversible process.
3. The storage of energy in a water-containing geologic material is mediated by the "hydraulic capacitance" parameter, which is conceptually analogous to "thermal capacitance" of the heat flow process. In general, hydraulic capacitance of a chunk of geologic material is the mass of water it can take into storage per unit change in water pressure. Because groundwater systems comprise deformable and desaturable geologic materials, the storage of energy involves mechanisms other than the elastic attributes of water. Thus, hydraulic capacitance includes effects due to mechanical deformation of the porous medium as well as the capillary potential of porous media.

SELF-ORGANIZATION TENDENCY OF A TRANSIENT SYSTEM

Given these attributes, how may one expect the system to optimize itself in response to forces which cause it to change its state over a small interval of time Δt?

A groundwater system which changes its state over a finite interval of time will experience a continuous expenditure of energy as water is moved through it. The energy so expended may come

either from the reserves already existing within the system or from influx of energy brought in by water moving into the system across boundary segments. Thus, there exists a continuous interaction between energy storage and energy expenditure during the transient flow process. Consequently, a tendency for self-organization, should one exist, could be reasonably expected to be related to how the system strikes a balance between storing energy and expending energy.

<u>POSTULATE 4:</u> Tendency for self-organization during change of state

During the transient process of water movement, the groundwater system tends to partition energy in some optimal way between reversible storage and irreversible mechanical work. By analogy with Hamilton's principle it is postulated that the difference between energy expended in doing work and the change in storage of energy is an extremum.

As before, consider that the flow system is divided into I = 1,2,3,4 ....., I flow tubes and j = 1,2,3,4, ..., J potential drops. The rate at which energy is expended in moving water over a small interval of time is equal to,

$$E_w = \text{Energy Expended as work} = \Delta t \left(\sum_i \sum_j \frac{(\Delta\Phi_{ij})^2}{R_{ij}^2} \right) . \tag{13}$$

For reasons to be discussed later in the section on Hamilton's Principle, we define, in an ad hoc fashion, energy stored in a segment of the flow tube to be equal to the energy contained in the segment at the beginning of the time interval less an incremental change in energy. Thus,

$$(E_s)_{ij} = \text{Energy stored in segment ij} = C_{ij}\left((\Phi_0)_{ij}^2 - (\Phi_{ij} - (\Phi_0)_{ij})^2 \right) , \tag{14}$$

where, C_{ij} is the hydraulic capacitance of the segment ij (dimension, MT^2/L^2) , Φ_0 is the initial potential at the beginning of the time interval and Φ is the potential at the end of the time interval. Note that $C_{ij}(\Phi_0)_{ij}$ is the mass of water contained in segment ij at the initial time, and, $C_{ij}(\Phi_0)_{ij}^2$ is the energy contained in the segment at the initial time. Similarly, $C_{ij}[\Phi_{ij} - (\Phi_0)_{ij}]^2$ is the incremental change in energy, being the product of the change in mass times the change in potential over segment ij. For the transient flow system, the postulate of self-organization states that the difference between the energy expended and the energy stored must be an extremum. Thus, we have, for a small interval of time Δt,

(15) $$\Omega = \Delta t\left(\sum_i \sum_j \frac{(\Delta\Phi_{ij})^2}{R_{ij}^2}\right) - C_{ij}\left((\Phi_0)_{ij}^2 - (\Phi_{ij} - (\Phi_0)_{ij})^2\right).$$

The implication is that as the system evolves over an interval of time Δt, Ω^* will be an extremum. By invoking infinitesimals we may express Ω in integral form as,

(16) $$\Omega = \int_0^{\Delta t}\int_V k^*(\nabla\Phi)^2 dV - \int_V c\left(\Phi_0^2 - (\Phi - \Phi_0)^2\right)dV ,$$

where c denotes hydraulic capacitance per unit volume.

The last expression for Ω is a variational statement of the transient groundwater flow process. That it reduces to the parabolic equation upon minimization is demonstrated in Appendix 2.

It is pertinent here to compare the above integral with the variational statement of the heat conduction equation proposed by Gurtin(1964),

(17) $$\Omega_{Gurtin} = \int_V \left(K * \nabla\Phi * \nabla\Phi + c * \Phi * \Phi - 2c * \Phi_0 * \Phi\right)dV ,$$

where the asterisks denote convolution in time. Because of the convolutions involved, Gurtin's variational statement does not explicitly involve time. Purely from a mathematical perspective, Gurtin showed that the minimization of the integral yields the parabolic partial differential equation. If we replace convolution by simple multiplication and recognize that

(18) $$(\Phi - \Phi_0)^2 - \Phi_0^2 = \Phi^2 - 2\Phi_0\Phi ,$$

then, we recognize that the variational statement derived from the self-organization postulate and Gurtin'c variational statement are quite similar.

ANALOGY WITH HAMILTON'S PRINCIPLE

In the early eighteenth century, Hamilton provided a logical basis to understand the behavior of dynamical systems. Hamilton's methodology can be understood in terms of three components, namely, the Hamiltonian, the Lagrangian and Hamilton's principle (Ballentyne and Lovett (1980)). In a conservative system (that is, a system which does not experience any external forces; Seale, 1977) consisting of many particles in motion, the Hamiltonian, H, is defined as,

(19)
$$H = T + V,$$

where, T is kinetic energy and V is potential energy. It is assumed that H can be expressed in terms of momenta and coordinates.

The Lagrangian (also known as kinetic potential) is the difference between kinetic energy and potential energy expressed in generalized coordinates. Unlike the Hamiltonian, the Lagrangian is applicable to non-conservative systems, that is, systems subjected to external forces (Seale, 1977). Thus, the Lagrangian is defined as ,

(20)
$$L = T - V .$$

Hamilton's principle states that in a dynamical system composed of discrete material particles and in which T and V are known as a function of coordinates and time, the integral,

(21)
$$\Omega_{\text{Hamilton}} = \int_{t_1}^{t_2} (T - V)\, dt$$

is as small as possible. That is, as the system evolves over time interval, it evolves in a fashion which minimizes (21). Note that Ω_{Hamilton} is merely the Lagrangian integrated over the domain of interest. It is of interest to compare the variational statement developed from Postulate 4 above with the logical format of Hamilton's principle for dynamical systems.

In view of (13) and (14), we may define the total energy in the system to be the sum of the energy stored and the energy expended. Thus,

(22)
$$H^* = E_w + E_s .$$

Similarly, the difference between energy expended and energy stored is,

$$L^* = E_w - E_s \quad . \tag{23}$$

And, the integral of L^* over an interval of time is (16), the variational statement of transient groundwater flow. We see that H^* is similar to H, L^* is similar to L and (16) is similar to (21). Thus, the logical structure of the development of the variational principle for transient groundwater flow is similar to that of the Hamiltonian, the Lagrangian and Hamilton's principle.

Caveat

The fact that the approach based on Postulate 4 led to a variational statement similar to Gurtin's mathematically derived variational principle and that the over-all structure of the development has similarities to that of Hamilton's principle are encouraging. However, caution is in order.

Note that in considering the energy stored in a chunk of geologic material over an interval of time we defined it as the sum of sum of the energy stored at the initial time less an incremental change in storage (14). That is,

$$E_s = C[(\Phi_0)^2 - (\Phi - \Phi_0)^2] \quad , \tag{24}$$

where C is the hydraulic capacitance of the chunk of material. However, intuition indicates that energy stored over an interval of time is in fact the difference between the energy content at the end and at the beginning of the time intervals,

$$E_{s,actual} = C[\Phi^2 - \Phi_0^2] \quad . \tag{25}$$

Although (25) is intuitively a more meaningful definition for stored energy, it is mathematically unsuitable in deriving the variational principle because a variational principle so constructed will not lead to the classical differential equation upon minimization. Thus, in trying to make physical sense out of the variational principle, one has two alternatives to consider. First, assuming that the differential equation is logically sound, one may seek a reason why (24) is indeed a correct expression for stored energy and is thus to be preferred over (25). Or, second, one may choose (25) in preference to (24) and formulate a variational statement which may have to be used purely as an integral and not compatible with the differential equation. This raises the possibility that dynamic groundwater systems may be understood logically in terms of hitherto untested integral equations.

OTHER INTRIGUING ISSUES

ADEQUACY OF MASS CONSERVATION APPROACH

Traditionally we have been trained to solve problems of groundwater dynamics in terms of the principle of mass conservation which is implicit in the partial differential equation describing non-steady diffusion. However, with the introduction of variational calculus it was recognized that the dynamics of groundwater movement could be understood in terms of integrals. While this recognition came about on mathematical grounds, its physical significance had largely remained unnoticed. From the form of (15) and (16), it is easy to see that the variational integral actually is a statement of energy optimization and that the Hamiltonian is in reality a statement of energy conservation. Therefore, it stands to reason that in solving the dynamic groundwater flow problem, it is necessary that both energy conservation and mass conservation are assured. However, the classical differential equation only assures mass conservation and ignores energy considerations. A question then arises: is the solution obtained for the partial differential equation consistent with energy conservation?

A simple example illustrates how the differential equation may not assure energy conservation. Consider a groundwater system occupied by a single homogeneous material, completely isolated from the outside world. At time t = 0, the potential distribution within the system is non uniform. Thus, at t = 0, the system is not under equilibrium and, given sufficient time, the system will tend to a state of equilibrium at which the potential is the same everywhere; that is, the system will be under hydrostatic equilibrium. If c is the specific hydraulic capacitance of the material occupying the system, then, the total energy in the system and the total mass of water in the system are,

(26a) $$\text{Total Mass of Water at time zero} = \int_V c\,\Phi\,dV\text{, and,}$$

(26b) $$\text{Total Energy at time zero} = \int_V c\,\Phi^2\,dV$$

Then, the average potential (energy per unit mass) over the flow domain at t = 0 is,

(27) $$\bar{\Phi}(t=0) = \frac{\int_V c\,\Phi^2\,dV}{\int_V c\,\Phi\,dV}.$$

If we allow the system to equilibrate to a hydrostatic condition, what will be the hydrostatic potential? Note that during the process of equilibration, water moves from locations of higher potentials to locations of lower potentials. Energy will be taken from storage from those locations where potential decreases and added to those locations where potential increases. Since the system is isolated and no external sources of energy are available, the energy needed to overcome resistance and move water will have to be derived from within the system. Therefore, part of the energy released from locations of declining potential will be irretrievably expended to overcome frictional resistance and the rest will be stored at those locations where potentials are rising. If this logic is correct, the total energy (that is, the energy which will manifest itself in the form of the potential Φ) at $t = \infty$ will be less than that which existed at $t = 0$. But, the total mass of water is the same. Hence, the average potential, which is the hydrostatic potential at $t = \infty$, will be such that,

$$\bar{\Phi}(t=0) > \bar{\Phi}(t=\infty) \quad . \tag{28}$$

However, if we choose to evaluate the final hydrostatic state purely on the basis of mass conservation, as we traditionally do, we would not be accounting for the energy lost in overcoming resistive forces. Consequently, we will conclude that,

$$\bar{\Phi}(t=0) = \bar{\Phi}(t=\infty) \quad . \tag{29}$$

This issue of looking at transient water movement from the perspective of work appears to be quite important and needs further attention. If indeed energy availability is an important issue, then two different materials (say sand and clay) which start with identical initial conditions may proceed to different equilibrium states because of their differing ability to offer frictional resistance and to store energy.

VECTORIAL MECHANICS AND ANALYTICAL MECHANICS

It is pertinent here to recognize two broad lines along which the science of mechanics has developed since the late seventeenth century. The discussion below is largely from Lanczos (1970). The first is the branch of "vectorial mechanics" which starts directly from Newton's Laws of motion and takes into account all forces acting on a particle, whose motion is uniquely determined by these forces. The problems which are well-suited for vectorial treatment are essentially those

which can be handled with a rectangular frame of reference, since the decomposition of vectors in curvilinear coordinates is a cumbersome procedure even with advanced principles of tensor calculus.

The other branch, usually called "analytical mechanics" originated with Leibnitz, a contemporary of Newton. As described by Lanczos (1970), in analytical mechanics, the entire set of equations of motion can be developed from one unifying principle which implicitly includes all the equations. The principle takes the form of minimizing a certain quantity, the "action". Since the minimizing principle is independent of any reference system, the equations of analytical mechanics hold for any set of coordinates. This permits one to adjust the coordinates employed to the specific nature of each problem.

Whereas the classical partial differential equation of groundwater flow is based on vector mechanics, the integral approach presented in the foregoing pages conforms to the spirit of analytical mechanics. Experience with natural groundwater systems has shown that these systems are invariably characterized by complex, convergent and divergent flow patterns. They should be naturally amenable to analysis with the help of curvilinear coordinates rather than with the help of rectilinear systems. The main practical difficulty in using curvilinear coordinates is the handling of detailed geometric information specific to each problem. Indeed, this difficulty in harnessing geometric information has significantly contributed to the traditional attention given to problems of prescribed symmetry and the development of tensor calculus. However, the outlook in regard to curvilinear coordinates has undergone a radical change in the recent past. With the availability of powerful graphics software, handling of large amounts of geometric information and processing them rapidly is now a reality. Consequently, the time has now come for us to devote attention to the approach of analytical mechanics with the view to making practical use of directly solving integral equations pertaining to natural groundwater systems characterized by complex, convergent and divergent flow patterns directly in terms of curvilinear coordinate systems.

MEANING OF A MATHEMATICAL SOLUTION

In solving problems of groundwater hydrology, as in the case of many other physical systems, the phrase "mathematical solution" is generally considered to be synonymous with a closed-form solution to the partial differential equation. However, the identification of a framework of basic postulates and the existence of variational principles show that the notion of a mathematical solution must transcend the notion of a differential equation. Ultimately, the scientific methods we use are based on observationally established "laws" to which our physical systems must conform[2]. Therefore, "mathematical solution", as applied to the groundwater system, must involve system response compatible with the "laws" or "postulates" of Newton, Hamilton and Lagrange. Such being the

[2] In the case of abstract mathematical systems, axioms are analogous to the notion of laws of physical systems. In physical sciences and mathematics, laws and axioms constitute irreducible sets of assumptions which govern all interpretation

case, one could, in principle, directly solve the integral equations stemming from the postulates (or the variational principle) and solve the steady-state or dynamic groundwater flow problem, regardless of whether a differential equation exists or not.

This insight is of interest because it suggests a way of getting things done that is different from the one and only traditional way we have been used to. It is good to have alternatives. Perhaps, the computer revolution may even render this alternate way more advantageous than the traditional methods we are used to.

CONCLUDING REMARKS

In order to rationally understand physical processes such as groundwater flow, the standard scientific method is to set up conceptual-mathematical models, which are bestowed with specific attributes. Ideally, these attributes of the abstract model should have one to one correspondence with the attributes of the real system which the model helps to understand. The model, even in the most favorable circumstance, will only possess few of the attributes of the real system. Hence there will invariably exist an information gap between the model and the real world.

The differential equation is one such model. In the present work we have created another model involving integrals constructed on the basis of a framework of postulates. Instead of relying on gradients at points, the integrals rely on potential drops and resistances over finite regions of space. Careful look at the integrals, without concern for differentials, has led to some interesting insights.

The integrals stemming from the postulates involve energy and work while the traditional approach of the differential equation dedicates attention to mass conservation. Discussions presented above raise a question whether the solution generated for the differential equation will assure energy balance. If energy is not conserved, is the credibility of the differential equation model diminished? Is there a need to explore alternative models which will assure mass conservation as well as energy conservation?

ACKNOWLEDGMENTS

I am grateful to G.I. Barenblatt, Sally Benson, Eric Brown, Darryl Chrzan, L. R. Narasimhan, Genevieve Segol, Garrison Sposito and Chin Fu Tsang for review and critique of this manuscript. This work was supported partly by the Director, Office of Energy Research, Office of Basic Energy Sciences of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098 through the Earth Sciences Division of the Ernest Orlando Lawrence Berkeley National Laboratory.

REFERENCES

Ballentyne, D.W.G. and D.R. Lovett, 1980. A dictionary of named effects and laws in chemistry, physics and mathematics. Chapman and Hall, New York, 346 p.

Darcy, H., 1856. Détermination des lois d'écoulement de l'eau à travers le sable. Dalmont, V. Les Fontaines Publiques de la Ville de Dijon, 590-594.

Fourier, J., 1807. Propagation of Heat. Unpublished monograph Presented to the Institute de France.

Gurtin, M.E., 1964. Variational principles for linear initial value problems, *Quart. Appl. Math.*, 22 (3), 252-256.

Hubbert, M. K., 1940. The Theory of Groundwater Motion. *Jour. Geol.*, 48(8) (Part 1),25-184.

Lanczos, C., 1970. The Variational Principles of Mechanics, Dover Publications Inc., New York, Fourth Edition, 418 p.

Maxwell, J. C., 1888. Elementary Treatise on Electricity, Oxford at the Clarendon Press, Second Edition, 208 p.

Ohm, G. S., 1827. Die galvanische Kett, mathematische bearbietet, Pamphlet. English translation by W. Francis, "The galvanic circuit investigated mathematically", Van Nostrand Co., New York, 269 p., 1891.

Seale, R.L., 1977. Energy, in Encyclopedia Britannica, 6, 853.

Sokolnikoff, I. S. and R. M. Redheffer, 1966. Mathematics of Physics and Modern Engineering, McGraw Hill New York.

APPENDIX 1

Variational Principle for Steady groundwater flow

Show that, upon minimization, the integral,

(A1) $$\Omega_1 = \int_V k^* (\nabla\Phi)^2 ,$$

leads to the Laplace Equation, $\nabla \cdot k^* \nabla\Phi = 0$.

Let h be an admissible function which is continuous over the flow domain but vanishes over the boundary Γ. Let λ be a real number such that,

(A2) $$\bar{\Omega}_1 (\Phi + \lambda h) = \int_V k^* \left(\nabla\Phi \cdot \nabla\Phi + 2\lambda \nabla\Phi \cdot \nabla h + \lambda^2 \nabla h \cdot \nabla h \right) dV .$$

Need to show that,

(A3) $$\left[\frac{d\bar{\Omega}_1}{d\lambda} \right]_{\lambda = 0} = \nabla \cdot k^* \nabla\Phi = 0 .$$

Using Green's First Identity (Sokolnikoff and Redheffer, 1966),

(A4) $$2 \int_V k^* \nabla\Phi \cdot \nabla h \, dV = -2 \int_V h \nabla \cdot k^* \nabla\Phi \, dV + 2 \int_\Gamma h k^* \nabla\Phi \cdot n \, d\Gamma .$$

The surface integral on the right hand side of (A4) is zero because, by definition, h vanishes on the boundary. Therefore,

(A5) $$\left[\frac{d\bar{\Omega}_1}{d\lambda} \right]_{\lambda = 0} = -2 \int_V h \nabla \cdot k^* \nabla\Phi \, dV .$$

If Ω_1 is to be an extremum for non-zero values of h, the integrand (A5) must be equal to zero, and hence it follows that,

(A6) $$\nabla \cdot k^* \nabla \Phi = 0 .$$

APPENDIX 2

Variational Principle for Transient Groundwater Flow

Show that, upon minimization, the integral,

(A7) $$\Omega = \Omega_1 + \Omega_2 = \int_0^{\Delta t} \int_V k^* (\nabla \Phi)^2 dV + c \int_V \left((\Phi - \Phi_0)^2 - \Phi_0^2 \right) dV ,$$

leads tothe parabolic equation, $\nabla \cdot k^* \nabla \Phi - c\,(\partial \Phi / \partial t) = 0$.

Note that the first integral on the right hand side of (A7) has already been shown in Appendix 1 to lead upon minimization to $\nabla \cdot k^* \nabla \Phi$. We now proceed to minimize the second integral on the right hand side of (A7),

(A8) $$\Omega_2 = c \int_V \left(\Phi - \Phi_0)^2 - \Phi_0^2 \right) = c \int_V \left(\Phi^2 - 2 \Phi \Phi_0 \right) dV .$$

Again, let h be an admissible function and λ be a real number. Then, perturbation by λh leads to,

(A9) $$\bar{\Omega}_2 (\Phi + \lambda h) = c \int_V \left[\Phi^2 + 2 \lambda h (\Phi - \Phi_0) + \lambda^2 h - 2 \Phi \Phi_0 \right] dV .$$

Differentiating with reference to λ and setting $\lambda = 0$, we get,

(A9) $$\left| \frac{d\Omega_2}{d\lambda} \right|_{\lambda = 0} = 2c \int_V h (\Phi - \Phi_0) dV .$$

Combining (A4) and (A9) and noting that $\Delta t \to 0$ $(\Phi - \Phi_0)/\Delta t = \partial\Phi/\partial t$, we get,

$$\left[\frac{d\Omega}{d\lambda}\right]_{\lambda=0} = -2\int_V h\left[\nabla\cdot k^*\nabla\Phi - c\left(\frac{\partial\Phi}{\partial t}\right)\right]dV \quad . \tag{A10}$$

If Ω has to be an extremum for all non-zero h, then the integrand of (A10) must be zero. Therefore,

$$\nabla\cdot k^*\nabla\Phi - c\frac{\partial\Phi}{\partial t} = 0 \quad . \tag{A11}$$

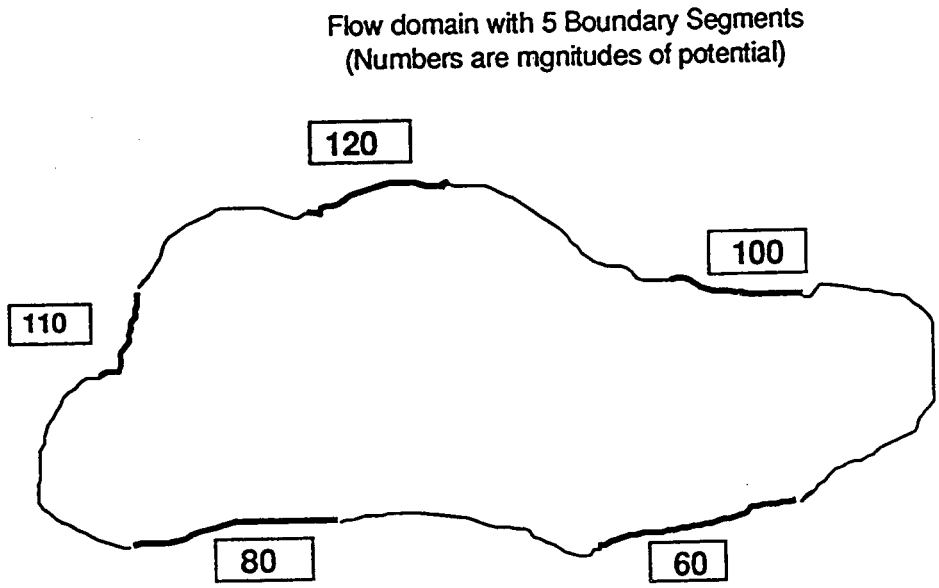


Figure 1: A flow domain with 5 boundary segments on which potentials are prescribed

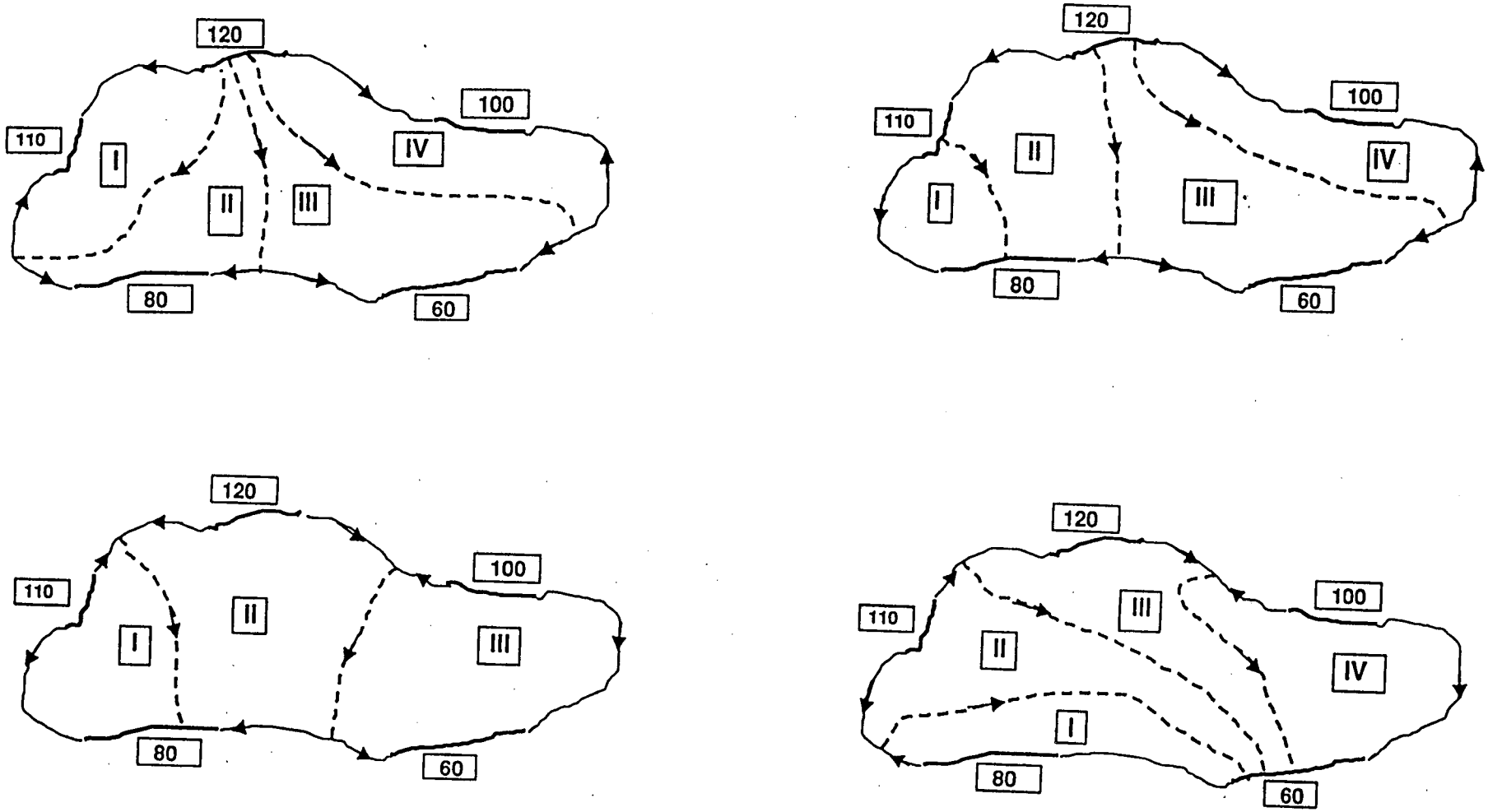


Figure 2: Four possible flow configurations, (A) One inlet and four outlets; (B) Two inlets and 3 outlets; (C) Three inlets and two outlets, and, (D) Four inlets and one outlet

Ernest Orlando Lawrence Berkeley National Laboratory
One Cyclotron Road | Berkeley, California 94720

Prepared for the U.S. Department of Energy under Contract No. DE-AC03-76SF00098