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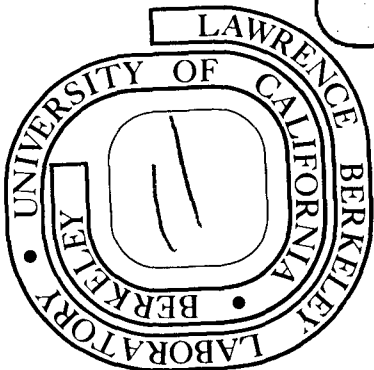
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ABSTRACT

In conceptualizing and quantifying the physical world of the porous medium, we are led to the consideration of properties averaged over finite subdomains. These averages are evaluated through some meaningful procedure of integration. In order that the physical significance of the averaging is assured, the procedure of integration must be consistent with the axiomatic foundations of integration and its relation to the nature of physical quantities. This paper points out the difference between extensive quantities (measures) and intensive quantities (potentials) and shows how the latter are to be first converted to the former before physically meaningful integration can be performed. The paper then proceeds to show how the averaging procedure can be simplified in special circumstances. The paper concludes with a consideration of how the volume-average of the conceptual-computational world can meaningfully simulate the physical world perceived through measurements.

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INTRODUCTION

In considering mass and energy transport through porous media, we encounter two types of physical properties. The first type which is of an extensive nature, includes mass and energy. Different from extensive properties are those properties which denote concentrations or intensities of mass or energy. These properties, independent of the quantity or shape of the porous medium are known as intensive properties and include as examples, temperature, pressure, density and porosity.

Mass and energy transfer in porous media occur in microscopic pores and are governed by physical phenomena interacting at that scale. However, quantified observations of mass and energy transfer in porous media are made on a much larger, macroscopic scale with the help of various measuring instruments. These instruments act as integrating devices and provide data meaningful in a statistical sense. As it happens, we have far greater ability to directly measure intensive physical properties than we have for measuring extensive properties. For example, fluid pressure and temperature (both intensive properties) are perhaps the most widely measured quantities in mass and heat transfer studies.

Using data statistically meaningful on a macroscopic scale, we first construct a conceptual model of the physical world in which intensive properties are placed in mutual, cause and effect relationships between each other on the foundation provided by the law of mass (or energy) conservation. We then proceed to implement the conceptual model

through a computational model in which we define averages over sub-regions of the porous medium which are larger than those sampled by the measuring devices. Thus, our understanding the physical world of the porous medium is very much related to averaging. A clear definition of what we wish to average and how we shall achieve the averaging is of fundamental importance.

The law of mass conservation, which constitutes the king-pin of the conceptual model is based on the simple concept of addition. Obviously, the quantity that is conserved must possess the additive property. Only extensive properties possess the additive property. Intensive properties do not.

Basic to the procedure of mathematical integration is the process of addition. That is, the integrand must possess the additive property. If we wish to perform integration that has physical meaning (e.g. conserve mass or energy over a part or whole of a porous medium) then the integrand must be a physical quantity possessing the required additive property.

The theory of sets and the associated concept of a measure (Narasimhan, 1976, 1978) provides the fundamental link between the physical world subject to the laws of mass and energy conservation and the conceptual-computational world of quantification. Properties such as mass, energy and volume are "set" functions defined over a set of spatial points. A "measure" is a set function which possesses the following properties: a) Its domain is the set of spacial points and whose range is the set of non-negative numbers, b) its value is zero over a null-set, and c) it possesses the additive property; that is, if f is a measure and A and B are two disjoint sets, then $f(A \cup B) = f(A) + f(B)$. We can easily see: a) that Mass and Energy are always positive in sign, b) that without space mass and energy do not exist, and c) that if A and B

are two disconnected subdomains of the porous medium then the mass or energy contained in subdomains A and B together is equal to the sum of the mass (or energy) in A plus the mass or energy in B. Despite their simplicity, (a), (b) and (c) are very important concepts and form the axiomatic foundation not only of the theory of integration, but also of the mathematical theory of transient transfer of mass and heat in porous media.

With the above elaborate introduction we now pass on to the consideration of volume-averaging.

VOLUME-AVERAGE

Given the spatial distribution of an intensive property of interest, the aim of volume-averaging is to evaluate the average value of the property over some macroscopic subdomain of the flow region. We seek to achieve this by integrating the property in some meaningful fashion over the subdomain. However, since an intensive property does not possess the additive property, it cannot be directly integrated. For the integration to be physically meaningful, the intensive quantity has to be converted to an extensive property or a measure. To this end, we introduce the concept of a "capacity" function which correlates an intensive quantity with a corresponding measure.

As an illustration, consider the familiar example of heat and temperature. For a unit volume of the flow region, defining c as the capacity function, we have

$$H - H_0 = \rho c(T - T_0) \quad (1)$$

where $(H - H_0)$ is the heat content of the unit volume element with reference to heat content at temperature T_0 , ρ is mass density, c is specific heat capacity defined as the heat energy required to change the temperature of a unit mass of the material by unity and T is the average temperature over the unit volume element.

Suppose we wish to evaluate the average temperature over some arbitrary subdomain ℓ of the porous medium over which the temperature distribution is known. Then we first divide the subdomain into the small volume elements dV , which are sufficiently large (non-microscopic) to permit a statistically meaningful definition of temperature. Next we compute the heat content over each dV using the capacity function and sum up the heat contents of all dV 's over the subdomain to obtain the heat content of ℓ . Finally, we define an average temperature for the subdomain by dividing its heat content by its heat capacity. Thus,

$$\langle T \rangle_{\ell} = \frac{1}{V_{\ell} \langle \rho c \rangle_{\ell}} \int_{V_{\ell}} \rho c T dV \quad (2)$$

where $\langle T \rangle_{\ell}$ is the average temperature over ℓ , V_{ℓ} is the volume of subdomain ℓ , $\langle \rho \rangle_{\ell}$ is the average density and $\langle c \rangle_{\ell}$ is the average specific heat of the material contained in ℓ .

Note that if the material contained in ℓ is heterogeneous or if ρ and c are functions of T , then, it is critical to properly define $\langle \rho \rangle_{\ell}$ and $\langle c \rangle_{\ell}$ in an appropriate fashion. As we shall see later, we could attempt to compute $\langle \rho \rangle_{\ell}$ and $\langle c \rangle_{\ell}$ by an averaging procedure analogous to (2). Or, perhaps more reliably, we may rely on experimental data to obtain these quantities.

We may point out here that the meaning of a subdomain as used here is quite flexible. Thus, if the subdomain ℓ is restricted to a particular phase (e.g. solid, liquid), then $\langle T \rangle_{\ell}$ is an average for that particular phase.

In groundwater hydrology, the most frequently measured intensive property is fluid pressure p while the measure of interest is mass of water. For a subdomain ℓ in a porous medium at a given average elevation one could relate $M_{w,\ell}$ and $\langle p \rangle_{\ell}$ with the help of the capacity

function $M_{C,\ell}^*$ as follows:

$$M_{W,\ell} = M_{C,\ell}^* \langle p \rangle_\ell + \text{constant} \quad (3)$$

where $M_{W,\ell}$ is the mass of water contained in ℓ . As defined by Narasimhan and Witherspoon (1977), $M_{C,\ell}^*$ is the fluid mass capacity of ℓ defined as the mass of water required to change the average pressure over ℓ by unity. In view of (3) and in a fashion analogous to (2), we can write:

$$\langle p \rangle_\ell = \frac{1}{V_\ell \langle m_C^* \rangle_\ell} \int_{V_\ell} m_C^* p dV \quad (4)$$

where $\langle m_C^* \rangle_\ell$ is the average specific fluid mass capacity of the material in ℓ and m_C^* is the specific fluid mass capacity of the material contained in dV defined as fluid mass capacity per unit volume of the porous medium. Here too, one could obtain m_C^* by averaging procedure or obtain it from experimental data.

It is of considerable interest to emphasize here that in setting up the conceptual equation of transient groundwater flow (e.g. Narasimhan and Witherspoon, 1977) we first evaluate the rate of accumulation of mass over a small volume element using divergence and then convert the rate of accumulation of mass to an equivalent change in potential by dividing it by its fluid mass capacity. The averaging procedure embodied in (4) is thus fully consistent with the concept of the non-steady diffusion equation.

SIMPLIFIED VOLUME AVERAGING

In (2) and (4) the capacity functions are different from unity. However, in the case of those intensive properties that are volume-normalized measures the capacity function is unity. Examples of this type of property include mass density, chemical concentration and porosity. For these properties, the volume average becomes much

simpler. Thus,

$$\langle \rho \rangle_{\ell} = \frac{1}{V_{\ell}} \int_{V_{\ell}} \rho dV \quad (5)$$

$$\langle \sigma \rangle_{\ell} = \frac{1}{V_{\ell}} \int_{V_{\ell}} \sigma dV \quad (6)$$

and $\langle n \rangle_{\ell} = \frac{1}{V_{\ell}} \int_{V_{\ell}} n dV \quad (7)$

where σ is concentration of a solute and n is porosity.

All volume normalized quantities, however, can not be volume-averaged in the simple fashion illustrated in (5), (6) and (7). For example, the quantity m_C^* denotes the mass of water required to change the average pressure over a unit volume by unity and is a volume normalized quantity. So also, is the product ρc which denotes the quantity of heat required to change the temperature of a unit volume of the material by unity. In these cases one is tempted to define

$$\langle m_C^* \rangle_{\ell} = \frac{1}{V_{\ell}} \int_{V_{\ell}} m_C^* dV \quad (8)$$

and

$$\langle \rho c \rangle_{\ell} = \frac{1}{V_{\ell}} \int_{V_{\ell}} \rho c dV \quad (9)$$

Yet, if we recall that m_C^* reflects the deformation and desaturation properties of the fluid filled porous medium and that $\langle \rho c \rangle$ reflects thermodynamic properties of materials, it is not clear whether the integrand in (8) or (9) can be considered to be additive from a physics view point especially if the material in ℓ is heterogenous. For example, if clay is interspersed as aggregates in sand, can one consider the

the compressibility of the bulk to be equal to the weighted sum of the compressibilities of sand and clay? Physically, there is reason to suspect that the deformation of the aggregated bulk may be quite complex and that for a given clay content two different aggregates may exhibit different deformation patterns. Therefore, a more meaningful method of obtaining volume averages of capacity functions may be to depend on carefully controlled field or laboratory experiments.

TRANSIENT AND STEADY FLOWS

Although, strictly speaking, volume averaging has to include the capacity coefficient within the integral sign many workers (e.g. Gray, 1975; Slattery, 1978; Pinder and Bear, 1978) define volume average by the simple expression

$$\langle \psi \rangle_{\ell} = \frac{1}{V_{\ell}} \int_{V_{\ell}} \psi dV \quad (10)$$

where ψ is any intensive property. Obviously, as a general definition of volume averaging (10) is not physically correct. However, (10) could be a valid expression under certain conditions. We will now consider this in some detail.

In the light of (5), (6) and (7), equation 10 could be valid if ψ is a property such as density, porosity or chemical concentration. Thus, in first condition under which (10) could be valid is that ψ is a volume-normalized measure.

A second possibility is that the material occupying the volume element V_{ℓ} has a constant value for the capacity coefficient. Thus, in (2) ρ and c are both constant over V_{ℓ} so that $\langle \rho \rangle_{\ell} = \rho$ and $\langle c \rangle_{\ell} = c$ and these quantities essentially cancel each other. Similarly, in (4), if m_C^* is constant over V_{ℓ} , then $m_C^* = \langle m_C^* \rangle_{\ell}$. In this case too,

the two quantities will cancel each other. Under these conditions, both (2) and (4) will simplify to the form of expression in (10).

A final possibility is that the flow system under consideration is characterized by steady flows and one is merely interested in the pattern of potential distribution arising due to known boundary conditions. Note carefully that the steady-state problem is independent of the capacity term since the quantity of mass or energy stored in the system does not change with time. Indeed, in considering the steady-state system if one chooses to neglect the actual quantity of mass or energy stored and concerns oneself only with the potential distribution, then one could assign any arbitrary, constant value for the capacity term over V_0 , thereby leading to a justification for using the expression (10) for volume-averaging.

The fact that many workers have persisted in using (10) as the fundamental definition of volume averaging leads to the inference that our approach to the physics of the problem is significantly influenced by our historical preference to the steady-state problem which is relatively more easy to solve than the transient problem.

A LINK BETWEEN MEASUREMENT AND MODELING

Having provided a physically meaningful definition of a volume-average we now consider its usefulness. The obvious first use of an average value of an intensive quantity over a volume is that one could multiply the average by the capacity of the volume element and compute the mass, energy or even the void volume stored in that element.

The second, most important use of the average value of an intensive quantity relates to the fact that gradients of intensive quantities give rise to forces which govern movement of fluids or heat. On a macros-

copie scale, these gradients depend on the spatial distribution of the average potential over subdomains. It is therefore necessary that the volume average of a potential computed for a given volume element be associated with a certain spatial location or point within the element.

Suppose the volume of the element V_ℓ is much larger than the volume δV which is the minimum size required for the property to be statistically meaningful. Then, if a measuring device is placed at a given point in V_ℓ it will presumably sample a volume δV and provide an average measurement of the property over δV . The important question now arises, what is the location of this point within V_ℓ such that the physically measured value at this point will equal the volume-averaged value over the element which is to be associated with this point?

Note, in this case, that V_ℓ is a conceptual element created to simulate the physical world and has to be, for convenience, larger than δV .

The exact location of the point at which the measured value equals the volume average clearly depends on the way the property varies over the element and the continuity of the variation. In general, as the spatial variation of the property changes with time, so will the location of the point. However, for computational purposes, it is extremely desirable that the point remains fixed in time. Under what conditions will the point remain fixed in space?

If we take the simple one dimensional case of a uniform material with constant capacity coefficient and consider a finite interval over which the property varies linearly, then we can verify without undue

difficulty that the volume average of the property will be exactly equal to the arithmetic mean, which, in turn, is equal to the value of the property exactly half way over the interval. Without offering a proof here, we could conjecture that in general two- or three-dimensions if V_ρ has arbitrary shape and if the desired intensive property varies linearly over V_ρ , the volume average will be equal to the magnitude of the property at the center of gravity of V_ρ .

If the aforesaid conjecture is true, then, by choosing V_ρ to be small enough to satisfy the linearity criterion and associating the volume average with the center of gravity, one could make the computational model consistent with the real world of observation. Indeed it appears that this linearity condition provides the vital link between the worlds of measurement and of modeling.

On the other hand if the capacity coefficient is variable over the element or if the intensive property varies non-linearly over the element, then as the shape of these variations change with time over the element, so also will the location of the point at which the physical measurement and volume averages coincide. Any errors in this regard will lead to inaccuracies in the evaluation of spatial gradients and consequently to errors in the evaluation of the diffusion equation. It is pertinent to point out here that the well-known finite element method often employs higher order (non-linear variations) approximations for the variation of potentials over finite subdomains of the flow region. Moreover, where the medium is heterogeneous, a single element of mass conservation may include more than one material with varying capacity coefficients, with the volume averaged quantities of the subdomain

associated with a point located at the junction of two or more different materials. In the light of the observations made earlier in this paragraph, it is easy to see that when dealing with transient flow problems the finite element approach can not always assure that the nodal point represents the point at which physical measurement and volume averages will coincide. To this extent, the foundations of the finite element scheme needs reconsideration for transient problems. However, for steady state problems, where the capacity function is unimportant, the finite element method, as it is employed now, is quite suitable. It is not out of place to mention here that the finite element method, as was originally introduced by structural engineers or even Galerkin's original paper, concerned itself strictly with the steady state problem.

SUMMARY AND CONCLUSIONS

Volume averages of intensive quantities are required in the conceptualization of heat and mass transfer problems. Integration is the fundamental tool employed in evaluating volume averages. Fundamental to integration is the additive property. Since intensive quantities are not additive, they ought to be first converted to extensive properties (measures) which possess the additive property. Capacity functions are functions which correlate intensive and extensive properties. These functions are essential components in the volume averaging process. The conventional definition of volume-averaging, in which several workers neglect the capacity coefficient, is valid only under certain limited circumstances. Notable among these is that the system is steady state and that one is not interested in the actual quantity of mass or energy stored in the system.

In addition to aiding in the estimation of the quantity of fluid stored within a volume element, volume averages also help in the evaluation of motion. In order that this could be achieved with least error, the volume element should be small enough so that the desired property varies linearly over it. In this case, if the capacity function is constant over the element, the volume average can be associated with center of gravity of the element. The linearity criterion provides the vital link between the world of measurement and that of computation. If the property varies non-linearly within V_λ , then computational errors may occur which may be controlled only with extra effort.

The importance of the concept of measure in integration and its relevance to the diffusion equation was originally proposed by this author during early 1975 in informal communications to fellow researchers in the field. The idea was described in a report published by the Lawrence Berkeley Laboratory in 1976, which, with some slight changes, was published as a journal paper in 1978. Recently, Pinder (1979) correctly drew attention to the importance of the concept of an extensive property in integration and the related volume averaging procedure. Pinder's presentation suggested to the author that the time has apparently arrived to recognize the importance of the foundations of integration in modeling physical systems governed, among others, by the diffusion process. This recognition provided motivation for the present paper which has attempted to highlight some of the fundamental consequences associated with volume-averaging.

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NOTATIONS

A,B:	Set of spatial points	
c:	Specific heat capacity	$\frac{\text{Energy}}{[M][\text{Temp}]}$
$\langle c \rangle_{\ell}$:	Average value specific heat capacity over subdomain ℓ	$\frac{\text{Energy}}{[M][\text{Temp}]}$
f:	Set function	
H:	Heat content at temp T	[Energy]
H_0 :	Heat content at Temp T_0	[Energy]
$M_{C,\ell}^*$:	Fluid mass capacity of subdomain ℓ	$[LT^2]$
m_C^* :	Specific fluid mass capacity	$[T^2/L^2]$
$\langle m_C^* \rangle_{\ell}$:	Average value of specific fluid mass capacity over subdomain ℓ	$[T^2/L^2]$
$m_{w,\ell}$:	Mass of water in subdomain ℓ	[M]
n:	Porosity	
p:	Pressure	$[M/LT^2]$
$\langle p \rangle_{\ell}$:	Average pressure over volume element ℓ	$[M/LT^2]$
T:	Temperature	
T_0 :	Reference temperature	
$\langle T \rangle_{\ell}$:	Average temperature over subdomain ℓ	
U:	Union of sets	
V_{ℓ} :	Volume of element ℓ	L^3
σ :	Concentration	M/L^3
ψ :	Any intensive property	

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