CHAPTER 1

AXIOMATIC FORMULATION OF THE BASIC MODELS

1.1 MODELS

The general procedure for predicting the behavior of a system is *modeling*. In this process, models are built that are used to predict a system's behavior. A model of a system is a surrogate whose behavior mimics that of the system. Models come in two flavors: physically built and mathematical. The models used most extensively today are mathematical models, since they are the most versatile and inexpensive. In specific applications, mathematical models consist of computer codes that are easily adapted to accommodate changes in systems properties. Furthermore, the foundations and methods of application of mathematical models, as will be seen, possess remarkable conceptual unity and generality. These features have very important practical implications, because they lead to great economies of effort and resources.

Mathematical models integrate scientific and technological knowledge with the purpose of predicting system behavior. Such knowledge is, thereby, incorporated into the computational codes that the computers execute in model utilization. At present, mathematical models founded on numerical simulation permit the study of complex systems and natural phenomena that otherwise would be very costly, dangerous,

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or even impossible to study by direct experimentation. From this perspective the significance of mathematical and computational modeling is clear; it is the most efficient and effective method for predicting the behavior of both natural and artificial systems of human interest. Worldwide, mathematical models are used ,extensively in engineering and science, in endeavors as diverse as the oil industry, water supply, weather and climate prediction, automobile and aircraft manufacture, medical studies, economics, chemical studies, and astronomy.

1.2 MICROSCOPIC AND MACROSCOPIC PHYSICS

This book deals with models of *macroscopic physical systems*, which include many systems of engineering and science. For this purpose an axiomatic approach, which we discuss below, is used; this is the most effective procedure for achieving generality and conceptual unity [1-13]. In particular, the use of axioms will permit us to construct an efficient approach for getting acquainted with the most important models of science and engineering.

There exist two approaches to the study of matter and its motion: the *microscopic approach*, which studies molecules, atoms, and elemental particles; and the *macroscopic approach,* which studies and models large systems. Matter, when it is observed at the ultramicroscopic level, consists of molecules and atoms, which in turn are made up of even smaller particles, such as protons, neutrons, and electrons. Prediction of the behavior of ultramicroscopic particles is a microscopic approach and is the subject matter of *quantum mechanics*.

Predicting the behavior of very large systems, such as an oil reservoir or the atmosphere, which consist of exceedingly large numbers of molecules and atoms, is an inaccessible goal using the microscopic approach. Thus, for problems of practical importance in science and engineering, a macroscopic approach is the appropriate one. The *mechanics of continuous media* supplies the theoretical foundations of the latter approach. The basis for the axiomatic method applied to the mechanics of continuous media was established in the second half of the twentieth century by a group of scholars and researchers whose most conspicuous leaders were C. Truesdell and W. Noll [[17], [31]-[36]].

Many systems of interest in engineering, earth sciences, applied sciences and sciences in general require models based upon the mechanics of continuous media. Among them are models of civil engineering structures, soils and foundations, the Earth's crust and deep interior, blood flow, the mechanics of human bones, natural resource reservoirs such as those of oil and water (both, surface and groundwater), the atmosphere, climate and weather prediction, and many others.

To predict weather or climate by following the motion of each particle of the atmosphere is obviously impossible. However, by applying the concepts drawn from the mechanics of continuous media, computational and mathematical modeling has led to very impressive achievements and has treated a great diversity of problems of science and engineering. The theory of *macroscopic systems* can be applied not only to physical systems, but also to chemical and some biological systems as well. Using

the continuum approach, for example, it is possible to predict the movement and evolution of microscopic biopopulations. In this approach, microscopic individuals are ignored; instead, the populations are assumed to be continuously distributed in all the space they occupy.

The study of this wide variety of problems in a unified manner by means of what we described earlier as the *axiomatic approach* yields an enormous economy of effort in the teaching-learning process. Furthermore, this manner of teaching and learning is very valuable in research, because the associated unified formulation contains clues for the solution of many heretofore unforeseen problems.

Some descriptions of the axiomatic approach to the formulation of continuous mechanics are difficult for non-mathematical audiences to follow, so herein we make an effort to simplify presentation of this approach without unduly compromising rigor. In particular, the presentation is similar to that contained in reference [1], which takes this approach. An important difference, however, is that we will employ the *intensive properties* by volume instead of by unit mass, since this yields significant advantages in the development and applications of the theory. We will now consider further the two approaches to viewing the world around us: that is, the *macroscopic and microscopic perspectives*.

When matter is studied using the macroscopic viewpoint, bodies completely fill the space they occupy, so that no voids exist in them, in spite of the fact that when they are examined with the help of a microscope, that is, from the microscopic point of view, one encounters many interstices. Thus, from the macroscopic point of view, for example, water fills the receptacle that contains it, and our work desk is a continuous piece of matter perfectly and sharply delimited.

This macroscopic viewpoint is present in classical physics, especially in classical mechanics. Science has now advanced to the point where we recognize that matter is full of voids that our senses do not perceive, and also that energy moves in subatomic packets; that is, it is *quantized*. At first glance these two approaches to the analysis of physical systems, the microscopic and the macroscopic, seem to be contradictory; however, they are not only compatible but are actually complementary, and a relation between them can be established by means of *statistical mechanics*.

1.3 KINEMATICS OF CONTINUOUS SYSTEMS

Let us begin with a consideration of some fundamental concepts. In the theory of continuous systems, as noted above, *material bodies completely fill the physical space that they occupy*. A *body* is a set of particles that, at any given time, occupies a *domain* (in the sense that this word is used in mathematics [[6]]) of the physical space. The body (that is, the set of particles) will be denoted by $\mathcal{B}$ and the domain that it occupies at time t will be denoted by $B(t)$. As for the time t, it can be any *real number*, that is, any number lying in the interval $-\infty < t < \infty$. However, in most studies of physical systems, the period of interest is contained in a finite time interval.

Given a body $\mathcal{B}$, other bodies that satisfy the condition $\mathcal{B} \supset B$ (that is, that are contained in it) will be said to be *subbodies of* $\mathcal{B}$.

Our discussion now proceeds by first considering *one-phase continuous systems* only, in which case a basic assumption of the theory is that given a body $\mathcal{B}$ at any time $t \in (-\infty, \infty)$, at each point $\underline{x} \in B(t)$[1] of the domain occupied by the body at such a time there is one and only one *particle* representative of or identified with that point in the body. For dynamical systems, particles change position as time evolves; thus a first problem with which the kinematics of continuous systems must deal is the identification of particles at different times. This is a challenge because generally the *same particle will have different locations at different times.*

A piece of information that identifies a particle uniquely is its position at a given time: the initial time, for example. Although this is not the only approach to identifying a particle, it is a very convenient one and one that will be used in what follows unless explicitly stated otherwise.

Let $\underline{p}(\underline{X}, t)$ *be the particle's position vector at time* t; then if the particle X has been identified by means of its position $\underline{X}$ at the initial time ($t = 0$), the following identity is satisfied:

$$\underline{p}(\underline{X}, 0) \equiv \underline{X}. \tag{1.1}$$

The *vector coordinates* $\underline{X} \equiv (X_1, X_2, X_3)$ are referred to as the *material coordinates* of the particle, while the function $\underline{p}(\underline{X}, t)$ is the *position-function.* We frequently reserve the notation $\underline{x}$for the coordinates of the position of the particle in the physical space; then

$$\underline{x} = \underline{p}(\underline{X}, t). \tag{1.2}$$

The relationship presented in Eq. (1.2) is illustrated in Fig. 1.1.

Generally, $\underline{x} \neq \underline{X}$, unless $t = 0$, in which case Eq. (1.1) is fulfilled. Observe that Eq. (1.2) supplies an answer to the question: At time t, where is the position, in the physical space, of *particle* X? Another question that frequently occurs is: At time t, what particle is located at position $\underline{x}$ of the physical space? The answer to the latter question is

$$\underline{X} = \underline{p}^{-1}(\underline{x}, t). \tag{1.3}$$

At any given time, t, the function $\underline{p}(\underline{X}, t)$ of Eq. (1.2) defines a transformation of a three-dimensional physical (Euclidean) space into itself. The notation $\underline{p}^{-1}(\underline{x}, t)$ is used for the *inverse transformation* of $\underline{p}(\underline{X}, t)$. An example of the use of this transformation is presented in Fig. 1.2. The existence of $\underline{p}^{-1}(\underline{x}, t)$ is a basic axiom of continuum mechanics, sometimes referred to as the *axiom of bodies impenetrability*: For one-phase systems, two different particles cannot occupy the same position at any time. In particular, the trajectories of different particles cannot cross.

When the material coordinates are defined fulfilling Eq. (1.1), then the set $\mathcal{B}$ is the domain that the body occupies at the initial time, and $\underline{X} \in B(0)$ if and only if the particle belongs to the body. On the other hand, as time passes the position in the

[1]Note that an underline denotes a vector quantity.

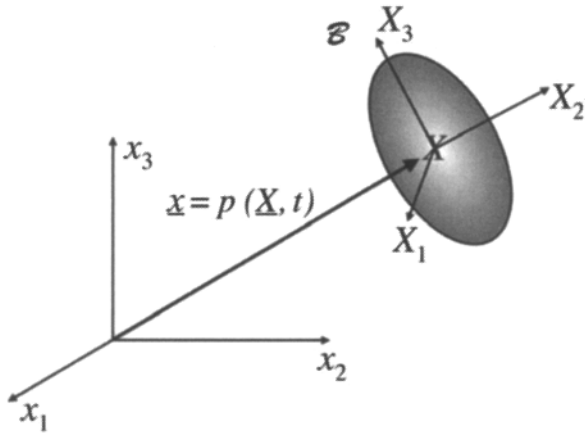

Figure 1.1 Relationship between material coordinates $\underline{X}$ and the coordinates of the position of the particle X in physical space $\underline{x}$.

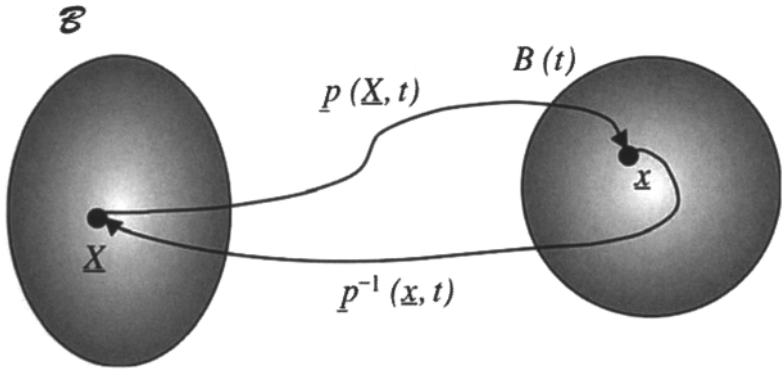

Figure 1.2 Relationship between the forward problem $x = \underline{p}\underline{X}, t)$ and the inverse relationship $\underline{X} = \underline{p}^{-1}\,(\underline{x}, t)$.

physical space of the body changes and $B(t)$ is the domain occupied by the body at any time t (see Fig. 1.2). In particular,

$$\mathcal{B} = B(0). \tag{1.4}$$

A formal definition of $B(t)$ is:

$$B(t) \equiv \left\{ \underline{x} \in R^3 \middle| \exists \underline{X} \in \mathcal{B} \ni \underline{x} = \underline{p}\,(\underline{X}, t) \right\} \tag{1.5}$$

which reads \a body B that is a function of time " is defined as follows: $\underline{x}$ is an element of R^3 such that there exists an $\underline{X}$ that is an element of $\mathcal{B}$ such that $\underline{x}$ is defined by the relationship $\underline{x} = \underline{p}\,(\underline{X}, t)$.

If a particle $\underline{X}$ is kept fixed while the time is varied, the function $\underline{p}(\underline{X}, t)$ yields the *trajectory of the particle*. In particular, the *velocity of a particle* is the derivative with respect to time of the function $\underline{p}(\underline{X}, t)$, when the choice of particle X is kept fixed. Thus, we define the *particle velocity* by

$$\underline{V}(\underline{X}, t) \equiv \frac{\partial \underline{p}}{\partial t}(\underline{X}, t). \tag{1.6}$$

1.3.1 Intensive properties

In continuum mechanics there is a class of functions, such as density or temperature, which have to be studied that are defined for each *particle* of a *body* and for each time. In general, any such function will be said to be an *intensive property*. When we consider an intensive property, we will write $\phi(\underline{X}, t)$ for its value at the particle location $\underline{X}$ at time t. This function, $\phi(\underline{X}, t)$, is said to be the *Lagrangian representation* of the intensive property.

On the other hand, one can consider this same intensive property from another point of view; let $\psi(\underline{x}, t)$ be the value of the intensive property at point $\underline{x}$ of the physical space at time t. The function $\psi(\underline{x}, t)$ is said to be the *Eulerian representation* of the intensive property. There is a condition that the Lagrangian and Eulerian representations of the same intensive property have to satisfy; it follows from Eq. (1.2) and is

$$\phi(\underline{X}, t) \equiv \psi(\underline{p}(\underline{X}, t), t) = \psi(\underline{x}, t). \tag{1.7}$$

In particular, the functions $\phi(\underline{X}, t)$ and $\psi(\underline{x}, t)$ are not the same. Furthermore, Eq. (1.7) implies that

$$\psi(\underline{x}, t) \equiv \phi(\underline{p}^{-1}(\underline{x}, t), t). \tag{1.8}$$

Clearly, Eqs. (1.7) and (1.8) are equivalent. The names we have adopted for these representations of intensive properties are to honor the mathematicians Leonard Euler (1707-1783) and Joseph-Louis Lagrange (1736-1813), respectively. The Lagrangian representation is used more frequently in the study of solids, while the Eulerian representation is more often used in the study of fluids. This is probably due to the fact that fluid displacements are usually very large, while displacements of solids are generally small.

Intensive properties may be scalar functions or vector functions. As an example, the particle velocity defined by Eq. (1.6) is a *vector-intensive property*. We notice that Eq. (1.6) yields the Lagrangian representation of the particle velocity. Also observe that a vector-intensive property is equivalent to three *scalar-intensive properties*: one scalar-intensive property for each component of the particle velocity.

In view of Eq. (1.7), the Lagrangian and Eulerian representations of the particle velocity satisfy

$$\underline{V}(\underline{X}, t) \equiv \underline{v}(\underline{p}(\underline{X}, t), t). \tag{1.9}$$

The Eulerian representation of the particle velocity, here denoted by $\underline{v}(\underline{x}, t)$, in view of Eq. (1.8) is given by

$$\underline{v}(\underline{x}, t) \equiv \underline{V}(\underline{p}^{-1}(\underline{x}, t), t). \tag{1.10}$$

The partial derivative with respect to time, $\partial\psi(\underline{x},t)/\partial t$, of the Eulerian representation of an intensive property is simply the rate of change of that property at a point that *remains fixed in the physical space*. On the other hand, the partial derivative with respect to time of the Lagrangian representation, $\partial\phi(\underline{X},t)/\partial t$, is, according to the definition of a partial derivative, the rate of change of such a property *that takes place at the particle under consideration as it moves in the space*; therefore, it is the rate of change that takes place at a point that moves in the physical space with the particle velocity. Or, to put this concept in more intuitive terms, it is the rate of change that we would observe if we rode on the particle and measured the intensive property.

It is useful to supply a formula for evaluating $\partial\phi(\underline{X},t)/\partial t$ in terms of the Eulerian representation, $\psi(\underline{x},t)$, of the property. Such a relationship can easily be derived from Eq. (1.7). Indeed, if we differentiate Eq. (1.7) with respect to time using the *chain rule*, we obtain, using Eq. (1.2),

$$\frac{\partial\phi(\underline{X},t)}{\partial t}=\frac{\partial\psi}{\partial t}(\underline{p}(\underline{X},t),t)+\sum_{i=1}^{3}\frac{\partial\psi}{\partial x_i}(\underline{p}(\underline{X},t),t)\frac{\partial p_i}{\partial t}(\underline{X},t) \tag{1.11}$$

or,

$$\frac{\partial\phi(\underline{X},t)}{\partial t}=\frac{\partial\psi}{\partial t}(\underline{p}(\underline{X},t),t)+\sum_{i=1}^{3}\frac{\partial\psi}{\partial x_i}(\underline{p}(\underline{X},t),t)V_i(\underline{X},t)\,. \tag{1.12}$$

Recalling Eq. (1.9) written in component form,

$$V_i(X,t)=v_i(\underline{p}(\underline{X},t),t). \tag{1.13}$$

Eq. (1.12) becomes

$$\frac{\partial\phi(\underline{X},t)}{\partial t}=\frac{\partial\psi}{\partial t}(\underline{p}(\underline{X},t),t)+\sum_{i=1}^{3}\frac{\partial\psi}{\partial x_i}(\underline{p}(\underline{X},t),t)v_i(\underline{p}(\underline{X},t),t) \tag{1.14}$$

or, more briefly,

$$\frac{\partial\phi(\underline{X},t)}{\partial t}=\frac{\partial\psi}{\partial t}(\underline{x},t)+\underline{v}(\underline{x},t)\cdot\nabla\psi(\underline{x},t)\,. \tag{1.15}$$

We will use the symbol $D\psi/Dt$ for the time derivative of the *Lagrangian representation*; it is given by

$$D\psi/Dt=\partial\psi/\partial t+\underline{v}\cdot\nabla\psi. \tag{1.16}$$

In particular, the acceleration of a *material particle*, $\underline{a}(\underline{x},t)$, is given by

$$\underline{a}(\underline{x},t)=(\partial\underline{v}/\partial t+\underline{v}\cdot\nabla\underline{v})(\underline{x},t) \tag{1.17}$$

or

$$a_i(\underline{x},t)=(\partial v_i/\partial t+\underline{v}\cdot\nabla v_i)(\underline{x},t)\,;\ i=1,...,3. \tag{1.18}$$

It follows from Eq. (1.6) that the Lagrangian representation of the acceleration is simply

$$\frac{\partial}{\partial t}\underline{V}(\underline{X},t)\equiv\frac{\partial^2}{\partial t^2}\underline{p}(\underline{X},t)\,. \tag{1.19}$$

1.3.2 Extensive properties

In this section we consider functions (that is, properties) that are *defined for each body of a continuous system*. This is to be contrasted with the functions (or properties) that we considered in the preceding section, which were defined for each material particle. We start with the definition of an extensive property: $E(\mathcal{B}, t)$ is said to be an *extensive property* when for every $\mathcal{B}$ it can be expressed as an integral of an intensive property over the body ; that is,

$$E(\mathcal{B}, t) \equiv \int_{B(t)} \psi(\underline{x}, t)\, d\underline{x}. \tag{1.20}$$

With respect to this definition, we note the following. Firstly, it is assumed that the Eulerian representations, $\psi(\underline{x}, t)$, of intensive properties to be considered in this section are integrable in the sense of *Lebesgue*.[2] Then, Eq. (1.20) establishes a one-to-one correspondence between extensive properties and intensive properties because the integrand function in Eq. (1.20) can always be taken as the definition of the Eulerian representation of an intensive property. Conversely, given an intensive property, its integral over each body defines an extensive property.

Second, the intensive property associated in this manner with each extensive property is the extensive property *per unit volume*. Note that in classical approaches (see, for example, reference [1]) intensive properties *per unit mass* have been used instead. However, the use of intensive properties per unit volume permits achieving greater theoretical consistency and more elegant developments. In particular, the correspondence between intensive and extensive properties is more direct. For example, when an extensive property is given by Eq. (1.20), its corresponding intensive property is the integrand in that equation.

In addition, when dealing with complicated systems such as multiphase and multicomponent systems, many masses may be involved in the systems and the application of formulas which use properties defined per unit mass may be confusing. On the other hand, the volume of the physical space is always uniquely defined.

It is also noteworthy that the computations required for transformation between the two definitions of intensive properties are easy to do: *The intensive property per unit volume equals the intensive property per unit mass multiplied by the mass density.*

Thus a paradox that the use of intensive properties per unit mass leads to is identified: When intensive properties are defined as the associated extensive property per unit mass and we try to be rigorous and systematic in the use of such a concept, the intensive property associated with mass (as an *extensive property*) is unity (so it is not density). Finally, calculus shows that

$$\psi(\underline{x}, t) \equiv \lim_{V \to 0} \frac{E(t)}{V} = \lim_{V \to 0} \frac{\int_{B(t)} \psi(\underline{\xi}, t)\, d\underline{\xi}}{V}. \tag{1.21}$$

[2]The main advantage of the Lebesgue integral approach over the more common Riemann integral approach is that more functions become integrable.

Equation (1.21) supplies an effective means for experimentally determining intensive properties (in the sense in which we have defined them and will be using them in what follows) associated with an extensive one: When the volume of the sample, V, is sufficiently small, the intensive property equals, approximately, the quotient of the extensive property divided by the volume of the sample.

A comment on notation: In Eq. (1.20) we have written $E(\mathcal{B}, t)$ for the extensive property, to emphasize that the extensive property is a function of the body $\mathcal{B}$ considered. However, to simplify the notation, from now on we will write simply $E(t)$, dropping $\mathcal{B}$, except in situations in which such a practice may create ambiguity.

On the other hand, we will use the concepts of intensive and extensive properties with considerable freedom, but always in a logically consistent manner. In particular, we will consider intensive and extensive properties as those that satisfy the conditions stated in the definitions of these concepts. It must be pointed out, however, that not every property that we may think of which satisfies such definitions will be physically relevant. That notwithstanding, the concepts of intensive and extensive properties are fundamental in the development of *continuum mechanics*, mainly because the basic models of continuous systems consist of balance equations of such properties.

1.4 BALANCE EQUATIONS OF EXTENSIVE AND INTENSIVE PROPERTIES

As said above, the basic mathematical models of continuous systems are formulated via balance equations operating on certain families of extensive properties. As an example, the models of solute transport (and the transport of contaminants by the atmosphere or by water in the surface or the subsurface are particular cases of this general kind of problem) are generated by carrying out the balance of the solute mass contained in every domain of the physical space. Here, the word *balance* is used in essentially the same sense as it is used in accounting. In accounting, the income minus the expenditure equals the net change in capital. Similarly, in continuum mechanics, the flux into minus the flux out of an extensive property equals its net change in this property.

1.4.1 Global balance equations

In order to calculate such balances it is necessary, first, to carry out an exhaustive identification of the possible causes by which the extensive property that is being considered may change. Let us take as an example the calculation of the balance of the number of automobiles that exist in a country. A simple analysis shows that there are only four possible causes for a change in such a number: Either automobiles are produced or destroyed in the interior of the country or they are imported or exported through its boundary (borders). In formulating our balance equation the concepts of producing, destroying, importing, and exporting must be used in a *mathematical* sense; that is, destroying (or junking) is *negative production*, while exporting is *negative importation*. Given this formalism, these two concepts completely cover all

possibilities of change. The balance equation becomes: *The net change in the number of automobiles in the country is due to the net production plus the net importation.*

To establish the balance equation of an extensive property, E, we will essentially follow the same steps as outlined above; the change in the extensive property, ΔE, will be given by

$$\Delta E = P + I. \tag{1.22}$$

Here, we have written P for the *production* of the extensive property in the interior of a domain of the physical space, and I for the *importation* of it through the boundary of such a domain.

Recalling that the *material particles* contained in a domain of the physical space constitute a body, we can use the ideas above to establish the balance equations that an extensive property of a body must fulfill. If we now introduce the concept of time, that is, the change in property E per unit time, we can use Eq. (1.22) to obtain

$$\frac{dE}{dt}(t) = \int_{B(t)} g\left(\underline{x}, t\right) d\underline{x} + \int_{\partial B(t)} q\left(\underline{x}, t\right) d\underline{x}. \tag{1.23}$$

The first integral is taken over the volume of the domain $B\left(t\right)$ and the second is taken over the surface $\partial B\left(t\right)$ of the domain $B\left(t\right)$. Here $g\left(\underline{x}, t\right)$ is called the *external supply of the extensive property, per unit volume and per unit time*; it represents the amount of the extensive property that enters the body, at point $\underline{x}$ and time t, per unit volume. As for $q\left(\underline{x}, t\right)$, *it represents the amount of the extensive property that enters the body through its boundary, at point $\underline{x}$ and time t, per unit area.* It can be shown, under very general conditions, that $q\left(\underline{x}, t\right)$is given by

$$q\left(\underline{x}, t\right) \equiv \underline{\tau}\left(\underline{x}, t\right) \cdot \underline{n}\left(\underline{x}, t\right). \tag{1.24}$$

Here, $\underline{n}\left(\underline{x}, t\right)$ is the *unit normal vector* on $\partial B\left(t\right)$, pointing toward the exterior of the body. The vector $\underline{\tau}$ is the *flux* of the *extensive property*. Using this relation, the balance represented by Eq. (1.23) can be rewritten as

$$\frac{dE}{dt}(t) = \int_{B(t)} g\left(\underline{x}, t\right) d\underline{x} + \int_{\partial B(t)} \underline{\tau}\left(\underline{x}, t\right) \cdot \underline{n}\left(\underline{x}, t\right) d\underline{x}. \tag{1.25}$$

This equation states that the rate of increase of property E in the body $B\left(t\right)$ is equal to the rate of introduction of property E introduced into the body $B(t)$ via an external supply plus the amount per unit time entering through the boundary $\partial B\left(t\right)$. This relationship is generally referred to as the *general equation of global balance*, which is a fundamental concept in the formulation of mathematical models of continuous systems.

1.4.2 The local balance equations

In this section we derive the *local balance equations*, which are expressed in terms of the intensive properties of continuous systems. The notation $\Sigma\left(t\right)$ will be used to denote a *shock*: that is, the surface across which the intensive properties are

discontinuous. In this notation the time t is included to make explicit that the shock position in the physical space generally depends on the time; that is, the shock generally moves. Standing shocks are included as particular cases of our general framework, just as the notation $f(\underline{x})$ in which the dependence on the argument $\underline{x}$ is made explicit includes as particular cases the constant functions.

The kind of discontinuities that may occur across $\Sigma(t)$ are jump discontinuities. We recall that, by definition, a *jump discontinuity* of a function is one in which the limits from each side of $\Sigma(t)$ exist but are different from each other. On $\Sigma(t)$ we define a *positive side* arbitrarily and then a unit normal vector pointing towards the positive side. Given a function, $f(\underline{x})$, with a jump discontinuity across $\Sigma(t)$, we define its *jump* and its *average*, respectively, by

$$[\![f]\!] \equiv f_+ - f_- \text{ and } \overset{\cdot}{\widehat{f}} \equiv \frac{1}{2}(f_+ + f_-). \tag{1.26}$$

Here f_+ and f_- stand for the limits of f on the positive and negative sides of $\Sigma(t)$, respectively.

Furthermore, due to the presence of *jump discontinuities* on the shock, concentrated sources also occur frequently on $\Sigma(t)$. Due to this fact Herrera introduced a more general form of the *equation of global balance* [[13],[15],[16]] of Eq. (1.25), that will be used throughout this book. It is

$$\frac{dE}{dt}(t) = \int_{B(t)} g(\underline{x},t)\,d\underline{x} + \int_{\partial B(t)} \underline{\tau}(\underline{x},t)\cdot\underline{n}(\underline{x},t)\,d\underline{x} + \int_{\Sigma(t)} g_\Sigma(\underline{x},t)\,d\underline{x}. \tag{1.27}$$

Here $g_\Sigma(\underline{x},t)$ represents an *external supply* that is concentrated on Σ.

The following lemma will be used later in our development.

Lemma 1 *-The general global balance equation, Eq.(1.27), is equivalent to*

$$\frac{dE(t)}{dt} = \int_{B(t)} \{g(\underline{x},t) + \nabla\cdot\underline{\tau}(\underline{x},t)\}\,d\underline{x} + \int_{\Sigma(t)} \{[\![\underline{\tau}]\!]\cdot\underline{n}(\underline{x},t) + g_\Sigma(\underline{x},t)\}\,d\underline{x}. \tag{1.28}$$

Proof: Under the assumption that the flux, $\underline{\tau}$, is piecewise continuous with jump discontinuities on $\Sigma(t)$, exclusively, Eq.(1.28) is derived by a straight-forward application of the generalized Gauss theorem described in the Appendix B. ∎

Next we present a mathematical result that also will be used later.

Theorem 2 *For each real number t, let $B(t) \subset R^3$ be a domain in which a body is located. Let $\psi(\underline{x},t)$ be a piecewise C^1 continuous intensive property [that is, C^1 except across $\Sigma(t)$]). Furthermore, let $\underline{v}(\underline{x},t)$ and $\underline{v}_\Sigma(\underline{x},t)$ be the particle velocity and the surface velocity of $\Sigma(t)$, respectively. Then*

$$\frac{d}{dt}\int_{B(t)} \psi\,d\underline{x} \equiv \int_{B(t)} \left\{\frac{\partial\psi}{\partial t} + \nabla\cdot(\underline{v}\psi)\right\} d\underline{x} + \int_{\Sigma(t)} [[(\underline{v}-\underline{v}_\Sigma)\psi]]\cdot\underline{n}\,d\underline{x} \tag{1.29}$$

Proof: *A proof is given in Appendix C.* ∎

Corollary 3 *Let $\psi(\underline{x}, t)$ be the intensive property that corresponds to the extensive property $E(t)$. Then*

$$\frac{dE}{dt} \equiv \int_{B(t)} \left\{ \frac{\partial \psi}{\partial t} + \nabla \cdot (\underline{v}\psi) \right\} d\underline{x} + \int_{\Sigma(t)} [[(\underline{v} - \underline{v}_\Sigma)\, \psi]] \cdot \underline{n}\, d\underline{x} \tag{1.30}$$

Proof: *Equations* (1.20) *and* (1.26) *together imply Eq.* (1.30). ∎

Corollary 4 *The general global balance equation, Eq. 1.27, is fulfilled, if and only if, for every body $B(t)$ the following relationship holds:*

$$\begin{aligned} &\int_{B(t)} \left\{ \frac{\partial \psi}{\partial t} + \nabla \cdot (\underline{v}\psi) - \nabla \cdot \underline{\tau}\,(\underline{x}, t) - g\,(\underline{x}, t) \right\} d\underline{x} \\ &+ \int_{\Sigma(t)} \{ [[(\underline{v} - \underline{v}_\Sigma) - \underline{\tau}]] \cdot \underline{n}\,(\underline{x}, t) - g_\Sigma\,(\underline{x}, t) \}\, d\underline{x} = 0. \end{aligned} \tag{1.31}$$

Proof: Equations. (1.28) and 1.30 together imply that

$$\begin{aligned} &\int_{B(t)} \left\{ \frac{\partial \psi}{\partial t} + \nabla \cdot (\underline{v}\psi) \right\} d\underline{x} + \int_{\Sigma(t)} [[(\underline{v} - \underline{v}_\Sigma)\, \psi]] \cdot \underline{n}\,(\underline{x}, t)\, d\underline{x} \\ = &\int_{B(t)} \{ g\,(\underline{x}, t) + \nabla \cdot \underline{\tau}\,(\underline{x}, t) \}\, d\underline{x} + \int_{\Sigma(t)} \{ [[\underline{\tau}]] \cdot \underline{n}\,(\underline{x}, t) + g_\Sigma \}\, d\underline{x}. \end{aligned}$$

∎

Theorem 5 *- Let $B(t)$ be a body. Then the global balance equation, Eq.(1.27), is fulfilled at every sub-body contained in $B(t)$ if, and only if, the following conditions are satisfied:*

1. The differential equation

$$\frac{\partial \psi}{\partial t} + \nabla \cdot (\underline{v}\psi) = \nabla \cdot \underline{\tau} + g, \text{ holds at every } \underline{x} \in B(t) - \Sigma(t). \tag{1.32}$$

2. The jump condition

$$[[\psi\,(\underline{v} - \underline{v}_\Sigma) - \tau]] \cdot \underline{n} = g_\Sigma, \text{ holds at every } \underline{x} \in \Sigma(t) \tag{1.33}$$

Proof: *That Eqs.(1.32) and (1.33) imply Eq.(1.31) is obvious. On the other hand, Eqs.(1.32) and (1.33) can be derived from the fact that Eq.(1.31) must be fulfilled for every subbody of $B(t)$.* ∎

The details of the proof of the latter result are left as an exercise at the end of this chapter.

In what follows, Eq. (1.32) will be referred to as the *differential equation of local balance*, while Eq. (1.33) will be the jump condition. It is timely to mention that

the differential equation of local balance is used more extensively than the jump condition. Indeed, practically all models of continuous media are based on Eq. (1.32), while the jump condition is used only when the model considered contains surfaces of discontinuity, and the latter situation seldom occurs. Nevertheless, a thorough discussion of continuous systems requires the study of the jump condition.

It is also useful to be acquainted with alternative expressions for the differential equation of local balance that are frequently used. In particular, each of the equations

$$\frac{\partial \psi}{\partial t} + \underline{v} \cdot \nabla \psi + \psi \nabla \cdot \underline{v} = \nabla \cdot \underline{\tau} + g \tag{1.34}$$

and

$$\frac{D\psi}{Dt} + \psi \nabla \cdot \underline{v} = \nabla \cdot \underline{\tau} + g \tag{1.35}$$

is equivalent to Eq. (1.32). For *stationary states* of continuous systems $\partial \psi / \partial t = 0$, Eq. (1.32) reduces to

$$\nabla \cdot (\underline{v}\psi) = \nabla \cdot \underline{\tau} + g. \tag{1.36}$$

Then, the jump condition presented in Eq. (1.33) becomes

$$[\![\psi \underline{v} - \underline{\tau}]\!] \cdot \underline{n} = g_\Sigma \text{ on } \Sigma(t) \tag{1.37}$$

since for stationary states one usually has $\underline{v}_\Sigma \equiv 0$.

1.4.3 The role of balance conditions in the modeling of continuous systems

As will be seen, associated with each model of a continuous system there is a unique family of extensive properties. Then the basic mathematical model of such a continuous system is constituted by the family of balance equations corresponding to each extensive property of the associated family, whose global formulations are given by Eq. (1.27). However, extensive properties are not used directly to express the local balance conditions; instead, such balances at the local scale are expressed in terms of their intensive properties. This substitution of extensive properties by their corresponding intensive properties is feasible because the global balance equation of Eq. (1.27) is equivalent to the local balance equations of Eqs. (1.32) and (1.33), and the latter do not involve extensive properties but rather their associated intensive properties.

The applicability of the local balance equations of Eqs. (1.32) and (1.33) is very wide since it includes models of continuous systems that contain surfaces of discontinuity. As noted earlier, such surfaces of discontinuity are frequently called *shocks*. Well-known examples of shocks are those that occur in supersonic flow of non-viscous compressible fluids. Other examples occur in hydraulics and in oil-reservoir mechanics. Shocks model very rapid changes that take place in the physical systems.

We observe that the local balance equations involve two kinds of relations that must be satisfied by the intensive properties: the balance differential equations and

the jump conditions; the former are differential equations that are fulfilled at every interior point of a body, while the latter are conditions to be fulfilled at the surfaces of discontinuity, or shocks. The use of Eq. (1.33) permits treating the shock phenomenon in a unified manner.

The balance differential equations, together with the jump conditions, constitute a *generic mathematical model*. In order for a generic model to acquire the capacity to predict behavior, it is necessary to incorporate in the model scientific and technological knowledge about the specific systems under consideration; this is achieved by means of *constitutive equations*. Once the constitutive equations have been combined with the balance differential equation, and the jump conditions, the problem of developing the model of the continuous system and deriving predictions from it becomes one that belongs to the fields of *partial differential equations* and *numerical methods*. Scientific computation, as used herein, supplies the methods and techniques required for applying the resulting mathematical model to specific problems of engineering and science.

1.4.4 Formulation of motion restrictions by means of balance equations

As a first application of the balance equations, in this subsection we formulate the conditions of *incompressibility of a fluid*, in two physical situations of practical interest: when the fluid is free to move in space and when it is contained in a porous medium.

The movement of a continuous system is said to be *isochoric* when every body of such a system conserves its volume. Clearly, the volume of a body is given by

$$V_B(t) \equiv \int_{B(t)} d\underline{x} = \int_{B(t)} 1 \, d\underline{x}. \tag{1.38}$$

When the movement is isochoric, one has

$$\frac{dV_B}{dt}(t) = 0. \tag{1.39}$$

Comparing Eqs. (1.38) and (1.39) with Eqs. (1.20) and (1.25), it is seen that in this case $\psi = 1$, as well as $g = 0$ and $\underline{\tau} = 0$. Substituting these values in the local balance differential equation, Eq. (1.32), one obtains

$$\nabla \cdot \underline{v} = 0. \tag{1.40}$$

This is the well-known *condition of incompressibility* that applies to a free fluid.

Assume now that we consider a fluid restricted to move in the pores, $V_v(t)$, of a porous medium (Fig. 1.3) and the question we would like to answer is: For a fluid contained in this porous medium, what are the conditions that the velocity satisfies when the motion is isochoric? The answer to this question is not as well known as that for a free fluid, but the question is answered as easily using the general scheme that we have already established. Consider the *volume of the pores* of the porous

medium. This is an extensive property because it can be written as an integral over the domain where the porous medium is located:

$$V_p(t) = \int_{B(t)} \varepsilon(\underline{x}, t)\, dx. \tag{1.41}$$

The integrand in this expression, $\varepsilon(\underline{x}, t)$, is the associated intensive property, known as *porosity*.It can be obtained in the laboratory by means of Eq. (1.21), which in this case yields

$$\varepsilon(\underline{x}, t) = \frac{\text{volume of voids}}{\text{total volume}}. \tag{1.42}$$

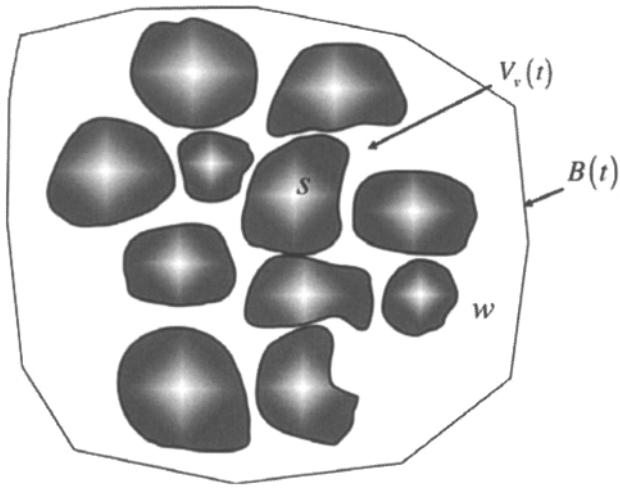

Figure 1.3 Diagrammatic representation of a porous medium. The medium is made up of solid s and water w.

A porous medium is said to be *saturated* by a fluid, w, when the pores are completely full of water; that is, when the volume of the fluid is equal to the volume of the pores. For isochoric motion of the fluid we can apply the general global balance equation, Eq. (1.27), taking as the extensive property the volume of the fluid (equal to the volume of the pores) with $g = 0$ and $\underline{\tau} = 0$ and $g_\Sigma = 0$. Therefore, the differential equation of local balance, Eq. (1.32), is

$$\frac{\partial \varepsilon}{\partial t} + \nabla \cdot (\varepsilon \underline{v}) = 0. \tag{1.43}$$

This equation is the *condition of incompressibility for a fluid contained in a porous medium*. Its physical meaning and application will be discussed in Chapter 5.

In subsurface hydrology and petroleum engineering the discontinuities of the porosity are most frequently associated with surfaces across which two different geological strata are in contact. Such surfaces are fixed in the physical space and,

therefore, $\underline{v}_\Sigma = 0$. Applying the jump conditions of Eq. (1.33), again with $\underline{\tau} = 0$ and $\psi = \varepsilon$, we get

$$[\![\varepsilon \underline{v}]\!] \cdot \underline{n} = 0 \text{ on } \Sigma. \tag{1.44}$$

This is the condition that the jump of the particle velocity of a fluid has to satisfy when the fluid goes from one geologic layer into another. The proof of the following algebraic identity is left as an exercise:

$$[\![\varepsilon \underline{v}]\!] = [[\varepsilon \underline{v}]] = [[\varepsilon]] \overset{\bullet}{\widehat{\underline{v}}} + \overset{\bullet}{\widehat{\varepsilon}} [[\underline{v}]]. \tag{1.45}$$

Using it, and Eq. (1.44), it is seen that

$$[[\underline{v} \cdot \underline{n}]] = -\frac{[[\varepsilon]]}{\overset{\bullet}{\widehat{\varepsilon}}} \overset{\bullet}{\widehat{v \cdot \underline{n}}}. \tag{1.46}$$

Therefore: *Whenever the porosity has a surface of discontinuity, the normal component of the particle velocity also has a discontinuity, which is proportional to its average.* The commonly used *Darcy velocity* is defined as

$$\underline{U} \equiv \varepsilon \underline{v}. \tag{1.47}$$

Using it, the jump condition of Eq. (1.44) can be written as

$$[\![\underline{U}]\!] \cdot \underline{n} = 0 \text{ on } \Sigma. \tag{1.48}$$

That is, the jump condition requires that the normal component of the Darcy velocity be continuous across surfaces of discontinuity of the porosity, albeit the normal component of the particle velocity is discontinuous there.

1.5 SUMMARY

Following a brief introduction to the scope of this book and the concept of modeling, we introduced several ideas that are central to understanding the material presented in later chapters. Representation of physical systems from microscopic and macroscopic perspectives was presented, followed by a consideration of the kinematics of continuous systems. An important aspect of this discussion was the identification of Eulerian and Lagrangian coordinate systems and their relationship to one another. The concepts of intensive and extensive properties were next presented and used to derive two equivalent formulations of the balance equations: one in terms of extensive properties (the global balance conditions) and the other in terms of intensive properties (the global local balance conditions). The chapter concluded with an application of the balance equations to formulate constraints in the motion of continuous systems.

EXERCISES

In each of the following two exercises, the motions of one-phase continuous systems are given by means of corresponding position functions $\underline{p}(\underline{X}, t)$. It is required to determine:

a. The initial particle positions

b. The function $\underline{p}^{-1}(\underline{x}, t)$

c. The Lagrangian representation of the particle velocity, $\underline{V}(\underline{X}, t)$

d. The Eulerian representation of the particle-velocity, $\underline{v}(\underline{x}, t)$

e. The Jacobian matrix of the motion:

$$\underline{\underline{J}}(t) \equiv \frac{\partial p_i}{\partial X_j}(\underline{X}, t) \tag{1.49}$$

1.1 The motion is given by

$$\begin{aligned} p_1(\underline{X}, t) &\equiv X_1 + t \\ p_2(\underline{X}, t) &\equiv X_2 + 3t \\ p_3(\underline{X}, t) &\equiv X_3 + te^{-t}. \end{aligned} \tag{1.50}$$

1.2 The motion is given by

$$\underline{p}(\underline{X}, t) \equiv \left(\|\underline{X}\|^2 + 3\|\underline{X}\|^{-1} t\right)^{\frac{1}{3}} \underline{X}. \tag{1.51}$$

1.3 The Lagrangian representation of the particle velocity of a one-phase continuous system is given by

$$\begin{aligned} V_1(\underline{X}, t) &= 3t \\ V_2(\underline{X}, t) &= \sin(2t) \\ V_3(\underline{X}, t) &= X_3. \end{aligned} \tag{1.52}$$

Assuming that the initial particle positions are taken as *material coordinates*, it is required to obtain

a) The *position function*, $\underline{p}(\underline{X}, t)$

b) The Eulerian representation of the *particle velocity*, $\underline{v}(\underline{x}, t)$

c) For the particle $\underline{X} = (1, 1, 0)$, a graphic of its trajectory in the time interval $0 \leq t \leq 1$

1.4 Let $\underline{p}(\underline{X}, t)$ be the position-function. The Lagrangian representation of the velocity is given by $V(\underline{X}, t) \equiv \frac{\partial p}{\partial t}(\underline{X}, t)$. Furthermore, let $\underline{v}(\underline{x}, t)$ and $\underline{a}(\underline{x}, t)$

be the Eulerian representations of the velocity and acceleration, respectively. It is required to establish:

a) The relation between $\underline{v}(\underline{x},t)$ and $V(\underline{X},t)$

b) The proof of the equation

$$\underline{a}(\underline{x},t) = \frac{\partial \underline{v}}{\partial t}(\underline{x},t) + \frac{1}{2}\nabla\left(v^2\right)(\underline{x},t) - \underline{v}(\underline{x},t) \times (\nabla \times \underline{v})(\underline{x},t)\,. \tag{1.53}$$

1.5 Let u and v be two piecewise-defined functions and Σ a surface where they have jump discontinuities. Prove that

$$[[uv]] \equiv (u_+v_+ - u_-v_-) = \dot{u}\,[[v]] + \dot{v}\,[[u]]\,. \tag{1.54}$$

Here

$$[[u]] \equiv (u_+ - u_-) \text{ and } \dot{u} \equiv \frac{1}{2}(u_+ + u_-) \tag{1.55}$$

and similarly for v. Using these relations, show Eq. (1.47). The equation

$$\frac{dE}{dt}(t) = \int_{B(t)} \left\{ \frac{\partial \psi}{\partial t} + \nabla \cdot (\psi \underline{v}) \right\} d\underline{x} \tag{1.56}$$

is a mathematical identity; when the domain of an integral depends on a parameter, t, it supplies an expression for the derivative with respect to such a parameter. It can be applied when

$$E(t) \equiv \int_{B(t)} \psi \, d\underline{x}. \tag{1.57}$$

A more intuitive form of this equation is

$$\frac{dE}{dt}(t) = \int_{B(t)} \frac{\partial \psi}{\partial t}\, d\underline{x} + \int_{\partial B(t)} \psi \underline{v} \cdot \underline{n}\, d\underline{x} \tag{1.58}$$

Prove that Eqs. (1.56) and (1.58) are equivalent. Furthermore, draw a figure to supply an intuitive interpretation of this result. To be valid , Eq. (1.51) requires that the function ψ be continuous. Show that when ψ is piecewise continuous, Eq. (1.51) must be replaced by

$$\frac{dE}{dt}(t) = \int_{B(t)} \frac{\partial \psi}{\partial t} d\underline{x} + \int_{\partial B(t)} \psi \underline{v} \cdot \underline{n}\, d\underline{x} - \int_{\Sigma(t)} [\![\psi \underline{v}]\!] \cdot \underline{n}\, d\underline{x} \tag{1.59}$$

1.6 Show that the following expressions for the differential balance equations are equivalent:

$$\frac{\partial \psi}{\partial t} + \nabla \cdot (\underline{v}\psi) = g + \nabla \cdot \underline{\tau} \tag{1.60}$$

$$\frac{\partial \psi}{\partial t} + \frac{\partial}{\partial x_j}(v_j \psi) = g + \frac{\partial \tau_j}{\partial x_j} \tag{1.61}$$

and

$$\frac{D\psi}{Dt} + \psi \nabla \cdot \underline{v} = g + \nabla \cdot \underline{\tau}. \tag{1.62}$$

1.7 Let $\Sigma(t)$ be a family of surfaces depending on the parameter t (time). Define $\underline{v}_\Sigma(t)$ as the velocity of the points on the intersection of such surfaces with the orthogonal trajectories to them. It can be seen that $\underline{v}_\Sigma(t)$ fulfills

$$\underline{v}_\Sigma = v_\Sigma \underline{n}. \tag{1.63}$$

Here $\underline{n}$ is a unit normal vector and v_Σ is a scalar. Assume that for each t, the equation of the surface is given by

$$F(\underline{x}, t) = 0. \tag{1.64}$$

Show that

$$v_\Sigma = -\left(\frac{\partial F}{\partial x_i}\frac{\partial F}{\partial x_i}\right)^{-\frac{1}{2}} \frac{\partial F}{\partial t}. \tag{1.65}$$

1.8 Assume that a porous medium is saturated by a fluid that conserves its mass. Adopt the notations $\varepsilon(\underline{x}, t)$, $\rho(\underline{x}, t)$, and

$$\underline{u} \equiv \varepsilon \underline{v} \tag{1.66}$$

for the porosity, density, and Darcy velocity of the fluid, respectively. The fluid volume is an extensive property, since it is given by

$$E(t) = \int_{B(t)} \varepsilon(t)\, dx. \tag{1.67}$$

Prove that it satisfies the following global balance equation:

$$\frac{dE}{dt}(t) = -\int_{B(t)} \varepsilon \frac{\partial \operatorname{Ln} \rho}{\partial t} dx. \tag{1.68}$$

Therefore:

a) When the fluid is incompressible:

$$\frac{\partial \varepsilon}{\partial t} + \nabla \cdot (\underline{u}) = 0. \tag{1.69}$$

b) When the fluid is compressible:

$$\frac{\partial \varepsilon}{\partial t} + \nabla \cdot (\underline{u}) = -\varepsilon \frac{\partial \operatorname{Ln} \rho}{\partial t}. \tag{1.70}$$

1.9 Show that there is one-to-one correspondence between extensive and intensive properties.

1.10 Prove Theorem 5 of Section 1.4.2 with details.

1.11 Prove that for each body, the change of body volume per unit volume per unit time equals the divergence of the particle velocity; that is, $\nabla \cdot \underline{v}$. In particular, when there is *mass conservation*, show that

$$\nabla \cdot \underline{v} = \frac{D\rho^{-1}}{Dt}.$$

1.12 Prove Eq. (B-8).

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