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Continuum versus Discrete Models

Introduction

Flow and transport phenomena in porous media and fractured rock as well as industrial synthetic porous matrices arise in many diverse fields of science and technology, ranging from agricultural, biomedical, construction, ceramic, chemical, and petroleum engineering, to food and soil sciences, and powder technology. Fifty percent or more of the original oil-in-place is left behind in a typical oil reservoir after the primary and secondary recovery processes end. The unrecovered oil is the main target for the enhanced or tertiary oil recovery methods now being developed. However, oil recovery processes only constitute a small fraction of an enormous and still rapidly growing literature on porous media. In addition to oil recovery processes, the closely related areas of soil science and hydrology are perhaps the best-established topics related to porous media. The study of groundwater flow and the restoration of aquifers that have been contaminated by various pollutants are important current areas of research. The classical research areas of chemical engineers that deal with porous media include filtration, centrifuging, drying, multiphase flow in packed columns, flow and transport in microporous membranes, adsorption and separation, and diffusion and reaction in porous catalysts.

Lesser known, though equally important, phenomena involving porous media are also numerous. For example, for the construction industry, the transmission of water by building materials (bricks or concretes) is an important problem to consider when designing a new building. The same is true for road construction where penetration of water into asphatene damages roads. Various properties of wood, an interesting and unusual porous medium, have been studied for a long time. Some of the phenomena involving wood include drying and impregnation by preservatives. Civil engineers have long studied asphalts as water-resistant binders for aggregates, protection of various types of porous materials from frost heave, and the properties of road beds and dams with respect to water retention. Biological porous media with interesting pore space morphology and wetting behavior include skin, hair, feathers, teeth and lungs. Other types of porous media that are widely used are ceramics, pharmaceuticals, contact lenses, explosives, and printing papers.

Flow and Transport in Porous Media and Fractured Rock, Second Edition. Muhammad Sahimi.

In any phenomenon that involves a porous material, one must deal with the complex pore structure of the medium and how it affects the distribution, flow, displacement of one or more fluids, or dispersion (i.e., mixing) of one fluid in another. Each process is, by itself, complex. For example, displacement of one fluid by another can be carried out by many different mechanisms which may involve heat and mass transfer, thermodynamic phase change, and the interplay of various forces such as viscous, buoyancy, and capillary forces. If the solid matrix of a porous medium is deformable, its porous structure may change during flow or some other transport phenomenon. If the fluid is reactive or carries solid particles of various shapes, sizes, and electrical charges, the pore structure of the medium may change due to the reaction of the fluid with the pore surface, or the physicochemical interaction between the particles and the pore surface.

In this book, we describe and study various experimental, theoretical, and computer simulation approaches regarding diffusion, flow, dispersion, and displacement processes in porous media and fractured rock. Most of the discussions regarding porous media are equally applicable to a wide variety of systems, ranging from oil reservoirs to catalysts, woods, and composite materials. We study flow phenomena only in a *static* medium, that is, one with a morphology that does not change during a given process. Thus, deformable media as well as those that undergo morphological changes due to a chemical reaction, or due to physicochemical interactions between the pore surface and a fluid and its contents, are not studied here. The interested reader is referred to Sahimi *et al*. (1990) for a comprehensive discussion of transport and reaction in evolving porous media and the resulting changes in their morphology.

1.1 A Hierarchy of Heterogeneities and Length Scales

The outcome of any given phenomenon in a porous medium depends on several length scales over which the medium may or may not be homogeneous. By homogeneous, we mean a porous medium with effective properties that are *independent* of its linear size. When there are inhomogeneities in the medium that persist at distinct length scales, the overall behavior of the porous medium is dependent on the rate of the transport processes, for example, diffusion, conduction, and convection, the way the fluids distribute themselves in the medium, and the medium's morphology. Often, the morphology of a porous medium plays a role that is more important than that of other influencing factors.

Consider, as an example, an oil reservoir, perhaps one of the the most important heterogeneous porous media. In principle, the reservoir is completely deterministic in that it has potentially measurable properties and features at various length scales. It could have been straightforward to obtain a rather complete description of the reservoir if only we could excavate each and every part of it. In practice, however, this is not possible and, therefore, a description of any reservoir, or any other natural porous medium for that matter, is a combination of the deterministic components – the information that can be measured – and indirect inferences that, by necessity, have stochastic or random elements in them. Over the past four decades, the statistical physics of disordered media has played a fundamental role in developing the stochastic component of description of porous media.

There are several reasons for the development. One is that the information and data regarding the structure and various properties of many porous media are still vastly incomplete. Another reason is that any property that we ascribe to a medium represents an average over some *suitably selected volume* of the medium. However, the relationship between the property values and the volume of the system over which the averages are taken remains unknown. The issue of a suitably selected volume reminds us that any proper description of a porous medium or fractured rock must have a length scale associated with it. In general, the heterogeneities of a natural porous medium are described at mainly four distinct length scales that are as follows (Haldorsen and Lake, 1984).

1. The *microscopic heterogeneities* are at the level of the pores or grains, and are discernible only through scanning electron microscopy or thin sections.
2. The *macroscopic heterogeneities* are at the level of core plugs, and are routinely collected in fields and analyzed. Such heterogeneities are found in every well with property values varying widely from core to core. In most theoretical studies, however, cores are assumed homogeneous and the average effective properties are assigned to them, notwithstanding their microscopic heterogeneities.
3. The *megascopic* or *field-scale heterogeneities* are at the level of the entire reservoir that may have large fractures and faults. They can be modeled as a collection of thousands, perhaps millions, of cores, oriented and organized in some fashion.
4. The *gigascopic heterogeneities* are encountered in landscapes that may contain many such reservoirs as described in the third example, along with mountains, rivers, and so on.

Not all of the aforementioned heterogeneities are important to all porous media. For example, porous catalysts usually only contain microscopic heterogeneities, and packed beds may be heterogeneous at both the microscopic and macroscopic levels. In this book, we consider the first three classes of heterogeneities and their associated length scales.

1.2 Long-Range Correlations and Connectivity

In the early years of studying flow phenomena in porous media and fractured rock, most researchers almost invariably assumed that the heterogeneities in one region or segment of the system were random and uncorrelated with those in other regions. Moreover, it was routinely assumed that such heterogeneities occur at length scales much smaller than the overall linear size of the system. Such assumptions were partly due to the fact that it was very difficult to model the system in a more realistic way due to the computational limitations and lack of precise experimental techniques for collecting the required information. At the same time, the simple conceptual models, such as random heterogeneities, did help us gain a better understanding of some of the issues. However, increasing evidence suggests that rock and soils do not conform to such simplistic assumptions. They exhibit *correlations* in their properties, and such correlations are often present at *all* the length scales. The existence of such correlations has necessitated the introduction of *fractal distributions* that tell us how property values of various regions of a porous medium depend on the length (or even time) scale of the observations, how they are correlated with one another, and how one can model such correlations realistically. Such concepts and modeling techniques are described in this book.

Once we accept that natural porous media and fractured rock are heterogeneous at many length scales, we also have to live with its consequences. As a simple, yet very important, example, consider the permeability of a porous medium, which is a measure of how easily a fluid can flow through it. In a natural porous medium and at large length scales (of the order of a few hundred meters or more), the permeabilities of various regions of the medium follow a broad distribution. That is, while parts of the medium may be highly permeable, other parts can be practically impermeable. If we consider a natural porous medium, then, the low permeability regions can be construed as the impermeable zones as they contribute little or nothing to the overall permeability, while the permeable zones provide the paths through which a fluid flows. Thus, the impermeable zones divide the porous medium into compartments according to their permeabilities. This implies that the permeable regions may or may not be connected to one another, and that there is disorder in the connectivity of various regions of the porous medium. Thus, if we are to develop a realistic description of a porous medium, the connectivity of its permeable regions must be taken into account.

The language and the tools for taking into account the effect of the connectivity of the permeable regions of a pore space are provided by *percolation theory*. Similar to fractal distributions, percolation has its roots in the mathematics and physics literature, although it was first used by chemists for describing polymerization and gelation phenomena. Percolation theory teaches us how the connectivity of the permeable regions of a porous medium affects its overall properties. Most importantly, percolation theory predicts that if the volume fraction of the permeable regions is below some critical value, the pore space is not permeable and its overall permeability is zero.

In the classical percolation that was studied over 50 years ago, it was assumed that the permeable and impermeable regions are distributed randomly and independently of each other throughout the pore space. Since then, more refined and realistic percolation models have been developed for taking into account the effect of correlations and many other influencing factors. Such ideas and concepts are developed and used throughout this book for describing various flow phenomena in porous media and fractured rock.

1.3 Continuum versus Discrete Models

Now that we know what kinds of heterogeneities one must deal with in studying porous media, it is also necessary to consider the types of models that have been developed over the past several decades for describing flow and transport phenomena in porous media and fractured rock. The analysis of flow, dispersion, and displacement processes in in porous and fractured media has a long history in connection with the production of oil from underground reservoirs. It was, however, only in the past 35 years that the analysis has been extended to include detailed structural properties of the media. Such studies are quite diverse in the physical phenomenon that they consider. In this book, we divide the models for flow, dispersion, and displacement processes in porous and fractured media into two groups: the *continuum models* and *discrete* or *network models*.

Continuum models represent the classical engineering approach to describing materials of complex and irregular geometry characterized by several distinct relevant length scales. The physical laws that govern flow and transport at the microscopic level are well understood. Thus, one can, in principle, write down differential equations for the conservation of momentum, energy, and mass and the associated initial and boundary conditions at the fluid-solid interface. However, as the interface in typical porous media is very irregular, practical and computationally and economically feasible techniques, while available, are often not feasible for solving such boundary-value problems – even when one knows the detailed morphology of the porous medium. Determination of the precise solid-fluid boundary remains a very difficult (if not impossible) task, particularly for large-scale porous media. The boundary within which one would have to solve the equations of change are so tortuous as to render the problem mathematically intractable. Moreover, even if the solution of the problem could be obtained in great detail, it would contain much more information than would be useful in any practical sense. Thus, it becomes essential to adopt a macroscopic description at a length scale much larger than the dimension of individual pores or fractures.

Effective properties of a porous medium are defined as averages of the corresponding microscopic values. The averages must be taken over a volume that is small enough compared with the volume of the system, but large enough for the equation of change to hold when applied to that volume. At every point in the medium, one uses the smallest such volume, thereby generating macroscopic field variables satisfying such equations as Darcy's law of flow or Fick's law of diffusion. The reasons for choosing the smallest suitable volume for averaging are to allow in the theory suprapore variations of the porous medium and to generate a theory capable of treating the usual macroscopic variations of the effective properties. In this book, we encounter several situations where the conditions for the validity of such an averaging are not satisfied. Even when the averaging is theoretically sound, the prediction of the effective properties is often difficult because of the complex structure of the pore space. In any case, with empirical, approximate, or exact formulae for the flow and transport coefficients and other effective properties, the consequences of a given phenomenon in a porous medium can be analyzed based on such a theory. As mentioned above, many of the past theoretical attempts to derive effective flow and transport coefficients of porous media from their microstructure entailed a simplified representation of the pore space, often as a bundle of capillary tubes. In this model, the capillaries were initially treated as parallel, and then later as randomly oriented. Such models are relatively simple, easy to use, and sufficiently accurate, provided that the relevant parameters are determined experimentally and the connectivity of the pore space does not play a major role. Having derived the effective governing equations and suitable flow and transport properties, one has the classical description of a porous medium as a continuum. We shall, therefore, refer to various models associated with the classical description as the continuum models.

The continuum models have been widely used due to their convenience and familiarity to the engineer. They do have some limitations, one of which was noted earlier in the discussion concerning scales and averaging. They are also not well-suited for describing those phenomena in which the connectivity of the pore space or the fracture network, or that of a fluid phase, plays a major role. Continuum models also break down if there are correlations in the system with an extent that is comparable with the linear size of the porous medium.

The second class of models, the *discrete models*, are free of the limitations of the continuum models. They have been advanced to describe phenomena at the microscopic level and have been extended in the last decade or so years to describe various phenomena at the macroscopic and even larger scales. Their main shortcoming, from a practical point of view, is the large computational effort required for a realistic discrete treatment of the pore space. They are particularly useful when the effect of the pore space or fracture network connectivity, or the long-range correlations, is strong. The discrete models that we consider in this book are mostly based on a network representation of porous media and fracture networks. The original idea for network representation of a pore space is rather old and goes back to the early 1950s, but it was only in the early 1980s that systematic and rigorous procedures were developed to map, in principle, any disordered porous medium onto an equivalent network. Once the mapping is complete, one can study a given phenomenon in porous media in great detail.

However, only in the past 35 years have ideas from the statistical physics of disordered media been applied to flow, dispersion, and displacement processes in porous and fractured media. The concepts include percolation theory, and fractal distributions and structures that are the main tools for describing the scale-dependence of the effective properties of disordered media and how long-range correlations affect them. What we intend to do in this book is to describe and review the relevant literature on the subject, define and discuss the ideas and techniques from the statistical physics of disordered media and their applications to the processes of interest in this book, and describe the progress that has been made as a result of such applications. In particular, we emphasize the important effect of the connectivity of the pores or fractures of a porous medium on the phenomena of interest. We also describe the characterization of fractured porous media and flow and transport in the fracture networks in great detail.

In summary, within this book we study models of porous media and fractured rock, explain various experimental techniques that are used for characterizing their morphology and flow and transport therein, describe the continuum models of flow and transport in such pore media, and compare them with the predictions of the discrete models. In all cases, we contrast the classical models and techniques with the modern approaches based on the discrete models. As such, we believe that the book is unique, as it treats the subjects of porous media and fractured rock on equal footing. We hope that this book can give the reader a clear view of where we stand in the middle of 2010.