LECTURE NOTES
IN PHYSICS

A. Hunt

Percolation Theory for Flow in Porous Media

With a Foreword by John Selker

Springer

Allen G. Hunt

Percolation Theory for Flow in Porous Media

Springer

Author

Allen G. Hunt
Department of Physics and Geology
Wright State University
Dayton, OH 45431
U.S.A.
Email: allenghunt@msn.com

Allen G. Hunt, *Percolation Theory for Flow in Porous Media*,
Lect. Notes Phys. 674 (Springer, Berlin Heidelberg 2005), DOI 10.1007/b136727

Library of Congress Control Number: 2005930812

ISSN 0075-8450
ISBN-10 3-540-26110-9 Springer Berlin Heidelberg New York
ISBN-13 978-3-540-26110-0 Springer Berlin Heidelberg New York

Springer is a part of Springer Science+Business Media
springeronline.com

Printed in The Netherlands

Typesetting: by the author using a Springer LaTeX macro package

Printed on acid-free paper SPIN: 11430957 54/Techbooks 5 4 3 2 1 0

Lecture Notes in Physics

The Lecture Notes in Physics

The series Lecture Notes in Physics (LNP), founded in 1969, reports new developments in physics research and teaching – quickly and informally, but with a high quality and the explicit aim to summarize and communicate current knowledge in an accessible way. Books published in this series are conceived as bridging material between advanced graduate textbooks and the forefront of research to serve the following purposes:

- to be a compact and modern up-to-date source of reference on a well-defined topic;
- to serve as an accessible introduction to the field to postgraduate students and nonspecialist researchers from related areas;
- to be a source of advanced teaching material for specialized seminars, courses and schools.

Both monographs and multi-author volumes will be considered for publication. Edited volumes should, however, consist of a very limited number of contributions only. Proceedings will not be considered for LNP.

Volumes published in LNP are disseminated both in print and in electronic formats, the electronic archive is available at springerlink.com. The series content is indexed, abstracted and referenced by many abstracting and information services, bibliographic networks, subscription agencies, library networks, and consortia.

Proposals should be sent to a member of the Editorial Board, or directly to the managing editor at Springer:

Dr. Christian Caron
Springer Heidelberg
Physics Editorial Department I
Tiergartenstrasse 17
69121 Heidelberg/Germany
christian.caron@springer-sbm.com

Foreword to Allen Hunt's First Book

Though a sledge hammer may be wonderful for breaking rock, it is a poor choice for driving a tack into a picture frame. There is a fundamental, though often subtle, connection between a tool and the application. When Newton and Leibniz developed the Calculus they created a tool of unprecedented power. The standard continuum approach has served admirably in the description of fluid behavior in porous media: the conservation of mass and linear response to energy gradients fit conveniently, and are solid foundations upon which to build. But to solve these equations we must characterize the up-scaled behavior of the medium at the continuum level. The nearly universal approach has been to conceive the medium as a bundle of capillary tubes. Some authors made the tubes porous, so they could fill and drain through their walls; others "broke and reconnected" them so each tube had a range of diameters along its length. In the end it must be admitted that the marriage of tool (capillary tube bundles) and task (to derive the constitutive relations for porous media) has not yet proven to be entirely satisfactory. Lacking in these conceptual models is a framework to describe the fluid-connected networks within the medium which evolve as functions of grain size distribution, porosity, saturation, and contact angle. This is fundamentally a geometry problem: how to concisely describe the particular nature of this evolving, sparse, dendritic, space-filling network.

Recognizing this basic problem, the community flocked to the fractal models as they became better understood in the 1990s. But fractals alone were not enough, as the real problem was to understand not the geometry of the medium, but the geometry of the fluids within the medium, and moreover, to correctly identify the geometry of the locations that control the flow.

I met Allen Hunt in the late 1990s, and over coffee he described his ideas about critical path analysis for the development of constitutive relationships for unsaturated conductivity. I was immediately sold: it was transparent that the geometric model (with the equally important framework for mathematical analysis) was ideally suited to the problem at hand. Since resistance to flow is a function of the fourth power of the pore aperture, clearly the key was to systematize the determination of the "weak link" to compute overall resistance to flow. Paths that had breaks were irrelevant; and paths that contained very small pores provided negligible contribution. The permeability should be proportional to the fourth power of the radius of the smallest pore in the connected path which has the largest small pore. Read that sentence twice: we are looking for the path of least resistance, and that path's resistance will be a function of the smallest pore in that path. Allen had the tool to identify this path as a function of fluid content. A very useful, appropriately sized, hammer had arrived for our nail. Over the following years Allen's work showed the power of using the right tool: he could explain the relationship between the geometry of the medium and liquid content versus permeability, residual fluid content, electrical resistance, diffusion of solutes, and even the thorny issues of the scale of a representative elementary unit. Critical path analysis is not a panacea, but due to the focus on the controlling geometric features, it provides a remarkably concise parameterization of fluid–medium relationships based on physically measurable properties that accurately predict many of the basic ensemble properties.

A fundamental problem in having these results be broadly understood and adopted is sociological. Consider how much time we spend learning calculus to solve the occasional differential equation. Critical path analysis requires calculus, but also understanding of the mathematics of fractals, and the geometric strategy of percolation theory. When Allen started his remarkably productive march into flow through porous media he deftly employed these tools that none of our community had mastered. There is a natural inertia to any discipline since re-tooling requires major investments of time. From this perspective I have long encouraged Allen to help the community make use of this essential set of tools by providing a primer on their application to flow though porous media. In this book Allen has once again moved forward strategically, and with great energy. He has provided an accessible tutorial that not only provides the bridge for the hydrologist to these new tools, but also the physicist a window into the specialized considerations of flow through natural porous media.

Learning new mathematical constructs is much like learning a new language. There is a great deal of investment, and the early effort has few rewards. Ultimately, however, without language there is no communication. Without mathematics, there is no quantitative prediction. If understanding the behavior of liquids in porous media is central to your work, I urge you to make the investment in learning this material. By way of this book Allen provides a direct and efficient avenue in this venture. Your investment will be well beyond repaid.

Corvallis, Oregon
April, 2005

John Selker

Preface

The focus of research in porous media is largely on phenomena. How do you explain fingering? What causes preferential flow? What "causes" the scale effect on the hydraulic conductivity? Why can the incorporation of 5% of hydrophobic particles into soil make the soil water repellent? Where do long tails in dispersion come from? These are merely a few examples of a very long list of questions addressed. The approach to "solving" problems is frequently to (1) take standard differential equations such as the advection–diffusion equation for solute transport, or Richards' equation for water transport; (2) substitute results for what are called constitutive relations such as the hydraulic conductivity, K, molecular diffusion constants, or air permeability as functions of saturation, and pressure-saturation curves, including hysteresis, etc.; (3) apply various models for the variability and the spatial correlations of these quantities at some scale; and (4) solve the differential equations numerically according to prescribed initial and/or boundary conditions. In spite of continuing improvement in numerical results, this avenue of research has not led to the hoped-for increase in understanding. In fact there has been considerable speculation regarding the reliability of the fundamental differential equations (with some preferring fractional derivatives in the advection–diffusion equation, and some authors questioning the validity of Richards' equation) while others have doubted whether the hydraulic conductivity can be defined at different scales.

Although other quite different approaches have thus been taken, let us consider these "constitutive" relations. The constitutive relationships used traditionally are often preferred because (1) they generate well-behaved functions and make numerical treatments easier; (2) they are flexible. This kind of rationale for using a particular input to a differential equation is not likely to yield the most informative solution. The most serious problem associated with traditional constitutive relations is that researchers use such concepts as connectivity and tortuosity (defined in percolation theory) as means to adjust theory to experimental results. But the appropriate spatial "averaging" scheme is inextricably connected to the evaluation of connectivity. In fact, when percolation theory is used in the form of critical path analysis, it is not the spatial "average" of flow properties which is relevant, but the most resistive elements on the most conductive paths, i.e. the dominant resistances on the paths of least resistance. An additional problem is that usual constitutive relations often cover simultaneous moisture regimes in which the represented physics is not equilibrium, and thus time-dependent, as well as those moisture regimes where the dominant physics is equilibrium, so that they must be overprescribed (while still not describing temporal effects). Finally, there has been no progress in making the distributions and spatial correlations of, e.g. K, consistent with its values at the core scale, because there is no systematic treatment of the connectivity of the optimally conducting regions of the system. This book shows a framework that can be used to develop a self-consistent and accurate approach to predict these constitutive relationships, their variability, spatial correlations and size dependences, allowing use of standard differential equations in their continuum framework (and, it is hoped, at all spatial scales).

Although applications of percolation theory have been reviewed in the porous media communities (e.g. Sahimi, 1993; Sahimi and Yortsos, 1990) (in fact, percolation theory was invented for treating flow in porous media, Broadbent and Hammersley, 1957) it tends to be regarded as of limited applicability to real systems. This is partly a result of these summaries themselves, which state for example that "Results from percolation theory are based on systems near the percolation threshold and the proximity of real porous rocks to the threshold and the validity of the critical relationships away from the threshold are matters of question," (Berkowitz and Balberg, 1993). However, it is well-known that percolation theory provides the most accurate theoretical results for conduction also, in strongly disordered systems far above the percolation threshold (using critical path analysis). The novelty in this course is the combined use of both scaling and critical path applications of percolation theory to realistic models of porous media; using this combination it is possible to address porous media under general conditions, whether near the percolation threshold or not.

This book will show how to use percolation theory and critical path analysis to find a consistent and accurate description of the saturation dependence of basic flow properties (hydraulic conductivity, air permeability), the electrical conductivity, solute and gas diffusion, as well as the pressure–saturation relationships, including hysteresis and non-equilibrium effects. Using such constitutive relationships, results of individual experiments can be predicted and more complex phenomena can be understood. Within the framework of the cluster statistics of percolation theory it is shown how to calculate the distributions and correlations of K. Using such techniques it becomes easy to understand some of the phenomena listed above, such as the "scale" effect on K, as well.

This work does not exist in a vacuum. In the 1980s physicists and petroleum engineers addressed basic problems by searching for examples of scaling that could be explained by percolation theory, such as Archie's law (Archie, 1942) for the electrical conductivity, or invasion percolation for wetting front behavior, hysteresis, etc. or by using the new fractal models for porous media. The impetus for further research along these lines has dwindled, however, and even the basic understanding of hysteresis in wetting and drainage developed in the 1980s is lacking today, at least if one inquires into the usual literature. In addition, the summaries of the work done during that time suggest that the percolation theoretical treatments are not flexible enough for Archie's law (predict universal exponents), or rely on non-universal exponents from continuum percolation theory without a verifiable way to link those exponents with the medium and make specific predictions. An identifiable problem has been the inability of researchers to separate connectivity effects from pore-size effects. This limitation is addressed here by applying percolation scaling and critical path analysis simultaneously. While there may have been additional problems in the literature of the 1980s (further discussed here in the Chapter on hysteresis), it is still not clear to me why this (to me fruitful) line of research was largely abandoned in the 1990s. This book represents an attempt to get percolation theory for porous media back "on track."

It is interesting that many topics dealt with as a matter of course by hydrologists, but in a rather inexact manner, are explicitly treated in percolation theory. Some examples are:

1. upscaling the hydraulic conductivity = calculating the conductivity from microscopic variability,
2. air entrapment = lack of percolation of the air phase,
3. residual water, oil residuals = critical moisture content for percolation, sum of cluster numbers,
4. grain supported medium = percolation of the solid phase;
5. Representative Elementary Volume = the cube of the correlation length of percolation theory,
6. tortuosity = tortuosity,
7. flow channeling = critical path.

These concepts and quantities are not, in general, treatable as optimization functions or parameters in percolation theory because their dependences are prescribed. Note that in a rigorous perspective for disordered systems, however, one does not "upscale" K. The difficulty here is already contained within the language; what is important are the optimal conducting paths, not the conductivities of certain regions of space. The conductivity of the system as a whole is written in terms of the rate-limiting conductances on the optimal paths and the frequency of occurrence of such paths. Defining the conductivity of the system as a whole in terms of the conductivities of its components is already a tacit assumption of homogeneous transport. Further, some elementary rigorous results of percolation theory are profoundly relevant to understanding flow in porous media. In two-dimensional systems it is not possible for even two phases to percolate simultaneously (in a grain-supported medium there is no flow or diffusion!), while in three dimensions a number of phases can percolate simultaneously. As percolation thresholds are approached, such physical quantities as the correlation length diverge, and these divergences cause systematic dependences of flow and transport properties on system size that can only be analyzed through finite-size scaling. Thus it seems unlikely that treatments not based on percolation theory can be logically generalized from 2D to 3D.

I should mention that a book with a similar title, "Percolation Models for Transport in Porous Media," by Selyakov and Kadet (1996) also noted that percolation theory could have relevance further from the percolation threshold, but overlooked the existing literature on critical path analysis, and never mentioned fractal models of the media, thereby missing the importance of continuum percolation as well. As a consequence, these authors did not advance in the same direction as this present course.

The organization of this book is as follows. The purpose of Chap. 1 is to provide the kind of introduction to percolation theory for hydrologists which (1) gives all the necessary basic results to solve the problems presented later; and which (2) with some effort on the part of the reader, can lead to a relatively solid foundation in understanding of the theory. The purpose of Chap. 2 is to give physicists an introduction to the hydrological science literature, terminology, experiments and associated uncertainties, and finally at least a summary of the general understanding of the community. This general understanding should not be neglected as, even in the absence of quantitative theories, some important concepts have been developed and tested. Thus these lecture notes are intended to bridge the gap between practicing hydrologists and applied physicists, as well as demonstrate the possibilities to solve additional problems, using summaries of the background material in the first two chapters. Subsequent chapters give examples of critical path analysis for concrete system models Chap. 3; treat the "constitutive relationships for unsaturated flow," including a derivation of Archie's law Chap. 4; hysteresis, non-equilibrium properties and the critical volume fraction for percolation Chap. 5; applications of dimensional analysis and apparent scale effects on K Chap. 6; spatial correlations and the variability of the hydraulic conductivity Chap. 7; and multiscale heterogeneity Chap. 8.

I wish to thank several people for their help in my education in hydrology and soil physics, in particular: Todd Skaggs, whose simulation results have appeared in previous articles and also in this book; John Selker, who showed me the usefulness of the Rieu and Sposito model for the pore space; Glendon Gee, who helped me understand experimental conditions and obtain data from the Hanford site; Eugene Freeman for providing additional Hanford site data; Bill Herkelrath, again for data; Toby Ewing, whose simulations for diffusion were invaluable; Tim Ellsworth for showing me the relevance of the experiments of Per Moldrup; Per Moldrup for giving me permission to republish his figures; Max Hu for providing me with his diffusion data; and

Sally Logsdon for her data on soil structure; Alfred Huebler for giving me a forum among physicists to discuss these ideas. I also thank my wife, Beatrix Karthaus-Hunt, for her support.

Dayton
April, 2005

Allen G. Hunt

Contents

1 Percolation Theory

1.1 What is Percolation?

Percolation describes properties related to the connectivity of large numbers of objects which individually have some spatial extent, and for which their spatial relationships are relevant and statistically prescribed.

Percolation theory comes in three basic varieties: bond, site, and continuum. We will consider all three varieties.

A simple bond percolation problem can be represented by a window screen which maps out a square grid (lattice). Consider cutting a fraction p of the elements of this grid at random. At some critical fraction $p \equiv p_c$, (which will turn out to be 0.5), the window screen will lose its connectedness and fall apart. Percolation theory addresses directly the question, "at what fraction of cut bonds does the screen fall apart," and related questions, such as, "what is the largest hole that can be found in the screen if some fraction of bonds less than the critical fraction is cut," and what the structure of such holes is. Percolation theory also readily answers the questions of what the electrical conductivity of such an incompletely connected network of (conducting) bonds is, or what the diffusion constant of a network of the same structure composed of water-filled tubes would be.

A simple site percolation problem can be represented by the random emplacement of metallic and plastic balls in a very large container. If two metal balls are nearest neighbors (touch each other) a current could pass from one to the other. If the number of metallic balls is high enough to reach a critical density, a continuous connected path through metal can be established. This path will conduct electricity. The larger the fraction of metallic balls, the better connected the path will be and the larger the electrical conductivity. Percolation theory generates the electrical conductivity as a function of the fraction of the balls made of metal. Site percolation problems can also be defined on grids.

A continuum percolation problem that had received attention already in the 1970's is a network of sintered glass and metallic particles. Such networks have analogues in the xerox industry. If the detailed structure is known, percolation theory can predict the electrical conductivity of these systems as well. The continuum percolation problem that we will be most interested in here is that of water flowing in variably saturated porous media.

Allen G. Hunt: *Percolation Theory for Flow in Porous Media*, Lect. Notes Phys. **674**, 1–31 (2005)
www.springerlink.com

In all of these variants of percolation theory it will be seen that the values of p_c vary widely from system to system, but that such relationships as those that give the size of the largest hole in the screen, or the conductivity, as a function of the difference between the fraction of cut bonds and the critical value, p_c, are universal, Stauffer (1979); Stauffer and Aharony (1994). Here universal means that the property is independent of the details of the system and depends only on the dimensionality, d, of the medium. The ultimate goal of this book is to demonstrate how percolation theory can be used to solve practical problems of transport and related properties of porous media. It has been hoped that the universal behavior near the percolation threshold could be used to guide understanding of real physical systems (for example, Berkowitz and Balberg, 1993; Sahimi, 1993; Sahimi and Yortsos, 1990). It has, however, also been pointed out more than once that it is not clear how close real systems are to the percolation threshold. Thus it is important to emphasize at the outset that this book will explain the use of percolation theory to calculate transport properties not merely near the percolation transition, but also far from it. The two methods have important differences. Far from the percolation transition it will be non-universal aspects of percolation theory, i.e. the value of p_c, which, together with the statistical characteristics of the medium, tend to dominate, while near the percolation transition it is the universal aspects that dominate. This perspective will be seen to be far more useful than a restriction to either case by itself, and it will be shown ultimately to allow calculation of all the transport properties of porous media, as well as their variability and the structure of their spatial correlations.

This first chapter is devoted to the development of basic methods and concepts from percolation theory with some concentration on those subjects most relevant to the applications. The material here is drawn from many sources, but most importantly from Stauffer (1979), Sahimi (1983) and Stauffer and Aharony (1994). The second chapter will serve as an introduction to problems and terminology of porous media. Subsequent chapters will detail the applications.

1.2 Qualitative Descriptions

Consider again a square grid of points and connect line segments between nearest neighbor points "at random." For very small values of p these segments will only connect pairs of nearest neighbor sites. As p increases more pairs will connect and gradually clusters of interconnected sites will appear. As p nears p_c many of these clusters will become large, and their internal structure will begin to be very complex. The perimeter (the number of connected sites with boundaries on the exterior of the cluster) has two contributions: one proportional to the volume (Kunz and Souillard, 1978), the second plays a role of a surface area and is proportional to the volume to the 1-1/d