

Preface

In recent years, the range and complexity of porous medium flow and transport problems of interest has increased dramatically. Problems in the environment involve water, gases, dissolved contaminants, and organic phases. They arise in agriculture, hydrology, and petroleum engineering in regions ranging from the deep subsurface to the near surface. In engineered systems, the behavior of filtration systems, fuel cells, and chemical reactors are described as porous medium systems. Other porous medium applications include diverse fields of study such as plant physiology, cancer tumor growth and treatment, and tomography. Interest in these problems has created a need to be able to describe multiphase problems with a relatively slow moving solid phase at a range of spatial scales. The thermodynamically constrained averaging theory (TCAT) has been developed to address this need.

TCAT is different from other scale-change methods because it assures full compatibility of problem descriptions at small scales and the larger length scales. Included in the analysis are formulations of dynamic equations for phases, interfaces between phases, common curves where interfaces come together, the geometric evolution of spaces occupied by and between phases, and thermodynamics. The larger scale descriptions are obtained in every case from averaging of smaller scale descriptions. These equations are then employed in their own right and used to formulate an entropy inequality that guides closure of the equations.

This book is an introduction to the TCAT framework. It contains all the elements of TCAT, but the applications considered are restricted to relatively simple cases. Because interscale consistency of all variables is mandated, significant explicit notation is employed to facilitate identification of the variables. Thus careful attention is paid to sorting through the subtleties of the notation so that the resultant equations can be seen to be both rigorous and meaningful.

The book consists roughly of two parts. The first half is focused on smaller scale continuum formulations of conservation and thermodynamic equations for phases, interfaces, and common curves. In the second half, tools for changing the scales of the equations are developed, the tools are used to derive foundational components of the theory, and the foundational components are used in turn to obtain closed models at a larger scale for a range of applications.

Specifically, Chap. 1 contains a qualitative overview of the elements of the TCAT method that will be employed quantitatively in the subsequent chapters. Chapters 2–5 are a self-contained presentation of principles needed for analyses at a length scale where phases are treated as being juxtaposed. Conservation equations for material in phases, interfaces, and common curves are developed in Chap. 2. These equations, applied to phases, are the ones usually encountered at a small continuum scale. The full dynamic equations for interfaces and common curves are an extension of the typical formulations. The conservation equations are developed for species that comprise an element of the system as well as for the elements as a whole. In Chap. 3, classical irreversible thermodynamics is developed for each of the constituents of a porous medium system. In Chap. 4, variational analysis is used to derive conditions of equilibrium for the system at the continuum scale. The variational techniques employed are derived in Appendix A. In Chap. 5, the equations and conditions developed in Chaps. 2–4 are combined to derive a closed equation set for a fluid phase. In this chapter, the approach to obtaining closure relations for a porous medium system is demonstrated, but by examining only a single fluid phase, the analysis is greatly simplified.

In Chaps. 6–11, the mathematical and physical considerations needed for analysis of systems at a larger scale, referred to as the macroscale, are provided. At this scale, the system is conceptualized as being composed of overlapping continua. In Chap. 6, the mathematical tools for scale change, derived in Appendix B, are applied to the conservation equations to obtain larger scale continuum equations. Averaging is applied in Chap. 7 to the thermodynamic relations, leading to a macroscale thermodynamic formalism that is unique to TCAT and fully consistent at the larger scale and between scales. The small scale equilibrium conditions of Chap. 4 are also averaged so that equilibrium conditions are expressed in terms of macroscale variables. In Chap. 8, evolution equations are developed to describe the volume fractions of each phase and other geometric variables that, on average, describe the distribution of phases within an averaging region. The changes in these variables, which do not exist at the smaller scale and cannot be described by conservation equations, are described based on averaging theorems. In Chaps. 9–11, examples are presented of application of the equations developed in Chaps. 6–8 to the description of porous medium systems: single-fluid-phase flow is considered in Chap. 9; chemical species transport in single-fluid-phase flow is developed in Chap. 10; and models for two-fluid-phase flow are derived in Chap. 11. The work in these latter three chapters to derive the desired forms requires substantial mathematical manipulations, which are detailed in Appendix C.

After working through these chapters, and the exercises at the ends of the chapters, one should have a firm grasp of the art and science of the TCAT approach. The method can then be applied by the reader to more complex systems. Chap. 12 presents a forward thinking discussion of some of the challenges and possibilities for confirming the mathematical descriptions that arise from TCAT and for supporting the discovery of parameter values in closure relations. Thus, we consider the entire text to be introductory in that it opens the door to systematic TCAT analysis and application but only hints at the applications that can be studied.

The methodologies described here have been developed by the authors with input obtained from many members of the scientific community. In particular, Professor D. Andrew Barry of EPFL has taken on the often difficult task of serving as journal editor for the reviews and publication of many of the research aspects of this work. The mostly anonymous authors of the thorough and challenging reviews that were obtained were very helpful in identifying aspects of the work that needed clarification and further development. We have been fortunate over the years to work with excellent students at the University of North Carolina (UNC) at Chapel Hill who both took our courses and contributed to the research. We also offered a series of short courses to students at the University of Stuttgart at the invitation of Professor Rainer Helmig, who has been an enthusiastic supporter of this work. Professor Helge K. Dahle of the University of Bergen has also provided encouragement for this work and opportunities to engage in enlightening and encouraging technical discussions on implementation of TCAT. These educational experiences, highlighted by the insights and commitment of students, encouraged us to develop TCAT so that it will be a more accessible analysis tool.

We have benefited from the efforts of additional collaborators. Professor Jan Prins of the Computer Science Department at UNC Chapel Hill has contributed expertise enabling the development of efficient, large-scale simulators of microscale systems. These simulators have been used to develop our mechanistic understanding and to support the functional forms of closure relations advanced in this work. The applied mathematics group at UNC Chapel Hill has supported this work intellectually and through numerical methods and analysis collaborations, especially Professors David Adalsteinsson, M. Gregory Forest, Jingfang Huang, and Richard McLaughlin. Professor Dorthe Wildenschild of Oregon State University has worked tirelessly to develop and apply high-resolution imaging methods that have informed our understanding and helped guide our theoretical work. Professor Laura J. Pyrak-Nolte of Purdue University has similarly contributed her expertise in micromodel experimental methods that have honed our thinking. Professor Tim Kelley and his group at North Carolina State University have contributed expertise in numerical methods to implement and evaluate TCAT models. Professor Bernhard A. Schrefler of the University of Padova has been an invaluable colleague, particularly in regard to solid mechanics and in implementing TCAT models for simulation of biological problems. Professor Kolumban Hutter, editor of the AGEM² series, has provided perceptive comments on our manuscript, and his unflagging and selfless support for this project is greatly appreciated.

The authors have made every attempt to eliminate typographical and conceptual errors and misstatements from the text. We are resigned to the fact that those efforts have not been completely successful. We acknowledge the heroic efforts of Ms. Robin Whitley in providing a careful proofreading of the text we prepared. Unfortunately, the authors retain ownership of all surviving typos, malapropisms, and stray notational markings.

The authors wish to acknowledge research funding that has been provided during the years it has taken to develop the TCAT methodology. In particular we wish to note support from the U.S. National Science Foundation, the Basic Energy Sciences

Program of the U.S. Department of Energy, and the Superfund Research Program of the U.S. National Institute of Environmental Health Sciences. The University of Bergen provided WGG an incomparable environment for working on this text using support obtained from the International Research Training Group Non-linearities and Upscaling in Porous Media (NUPUS) grant provided by the Norwegian Research Council and from a guest researcher grant through the University of Bergen Akademia agreement with Statoil. The University of North Carolina at Chapel Hill has provided support to CTM through his appointment as the Okun Distinguished Professor of Environmental Engineering and an environment that has enabled the completion of this effort.

The authors would be terribly remiss not to mention the supportive environments for this work encountered at home that involved many late nights, long weekends, and distractions from social duties. Environments unconstrained by averages, fostered by unlimited forbearance on the part of Genny Gray and Cherie Smith-Miller, were beyond any reasonable expectation and are more than gratefully appreciated.

Chapel Hill, NC
December 2013

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Introduction to the Thermodynamically Constrained
Averaging Theory for Porous Medium Systems

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2014, XXXIV, 582 p. 12 illus., 11 illus. in color.,

Hardcover

ISBN: 978-3-319-04009-7