

---

# 1 Multiscale Modeling of Porous Medium Systems

*Amanda L. Dye, James E. McClure,  
William G. Gray, and Cass T. Miller*

## CONTENTS

1.1	Introduction .....	3
1.2	Overview.....	5
1.3	Theory.....	6
1.3.1	Averaging Theorems.....	6
1.3.2	Conservation and Balance Equations .....	7
1.3.3	Entropy Balance .....	9
1.3.4	Thermodynamic Formalism.....	10
1.3.5	Evolution Equations.....	13
1.3.6	Entropy Inequality .....	15
1.4	Model Formulation .....	16
1.5	Microscale Considerations.....	18
1.6	Lattice Boltzmann Modeling.....	20
1.6.1	Formulation.....	20
1.6.2	Verification and Parameter Estimation.....	24
1.6.3	Validation.....	24
1.7	Computational Geometry Methods .....	27
1.8	TCAT Closure Relations.....	27
1.8.1	Simulations .....	27
1.8.2	Capillary Pressure–Saturation–Interfacial Area Relation.....	30
1.8.3	Disconnected Nonwetting Phase .....	32
1.8.4	Dynamic Relaxation .....	35
1.9	Discussion and Conclusions.....	37
	Nomenclature.....	38
	Acknowledgments.....	42
	References.....	42

## 1.1 INTRODUCTION

The use of computers over the last 60 years for simulating subsurface flow problems has provided an impressive, ever-expanding ability to model processes at a high resolution. Whereas in the 1960s a computational grid with 500 fixed nodes would have pushed the boundaries of computer power [59], simulations today involve millions of spatial grid points and adaptive meshes [40,57]. The availability of this power for solving equations that purport to describe physical and chemical processes in porous media is wasted, however, if the equations being used to describe