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RPPR Final Report
as of 21-Dec-2018

Agency Code:

Proposal Number: 65276MA **Agreement Number: W911NF-14-1-0287**

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Report Date: 30-Nov-2018 Date Received: 20-Dec-2018
Final Report for Period Beginning 06-Jun-2014 and Ending 31-Aug-2018
Title: Thermodynamically Constrained Averaging Theory for Multiscale Systems
Begin Performance Period: 06-Jun-2014 **End Performance Period:** 31-Aug-2018
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STEM Degrees: 0 **STEM Participants:** 2

Major Goals: The overall goal of this proposed work is to advance macroscale mathematical models of water resources systems. The specific objectives of this work are: (1) to formulate macroscale TCAT models for two-fluid-phase flow and species transport; (2) to advance TCAT theory to describe land-atmosphere interactions; (3) to advance TCAT theory to describe sediment transport in near shore surface water environments; (4) to advance microscale computational approaches to derive closure relations for macroscale models; (5) to implement macroscale simulators for novel classes of macroscale models; and (6) to validate restrictions, approximations, and overall macroscale model forms for varying classes of water resources models.

Accomplishments: Most objectives were accomplished and a new objective emerged during the project as a result of mutual interests with ERDC and unique capabilities in the area of entropy viscosity modeling. A brief summary is as follows:
1. A compositional model for two phase species transport was developed and published.
2. TCAT theory was advanced to model sediment transport and a manuscript is in review.
3. A great deal of work was accomplished to advance and apply microscale computational approaches and several publications have resulted from this work.
4. Macroscale models for non-dilute species transport have been developed, evaluated, and published.
5. Substantial work has been accomplished and published to close, evaluate, and validate macroscale closure relations.
6. Entropy viscosity methods have been developed for non-dilute species transport, the work presented, and a manuscript is in development.

Within these general areas, the team has actively worked, presented the work at many national and international meetings, and published essentially all of this material. Other publications resulting in part from this work will be published in the coming months.

Training Opportunities: This project provided support for one PhD student, Tim Weigand, who is in the final stages of writing his dissertation. Because of the theoretical nature of the work to derive new models, this work has catalyzed the research of several other students in the group as well, including a PhD student in mathematics who is now an employee of ERDC. The research was also used in several graduate courses populated by mathematics and geosciences students.

Results Dissemination: The results of this work have been disseminated to Army lab personnel at ERDC. This has included joint work, collaborative visits, and delivery of a seminar. Lattice Boltzmann software for simulating porous medium systems has been developed, run on some of the fastest computers in the world, and released as open source. This work has also been presented to a variety of applied audiences through invited and contribution presentations intended to disseminate, and distill, the high-impact results from this research to audiences that can benefit from the advances.

Honors and Awards: Co-PI William G. Gray was elected to the National Academy of Engineering based, in part, on his joint work with the PI on the development of the thermodynamically constrained averaging theory, which was further developed and applied in this grant.

Both Professors Miller and Gray delivered many invited lectures based upon the work performed on this project. Some examples include a lecture by Miller at the Gordon Research Conference on permeable media in July 2018, and lectures by both Miller and Gray at the ALERT graduate school workshop in France in October of 2017. Professor Miller also delivered invited lectures in Saudi Arabia at King Fahd University of Petroleum and Minerals, the Institute for Advanced Study in Munich, and the Department of Mathematics at the University of Padua all in October of 2018.

Protocol Activity Status:

Technology Transfer: Substantial and ongoing interaction with the ERDC lab occurred during this project, which resulted in several joint publications on TCAT model development and validation. Recently this work has included joint work on the development of entropy viscosity methods, which combine TCAT methods with numerical methods work underlying Proteus, a simulation environment developed by ERDC.

PARTICIPANTS:

Participant Type: PD/PI
Participant: Cass T. Miller
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Co PD/PI
Participant: William G. Gray
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: Y
Other Collaborators:

Participant Type: Co PD/PI
Participant: James E. McClure
Person Months Worked: 2.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)
Participant: Timothy M. Weigand
Person Months Worked: 12.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)
Participant: Brittany J Sphepherd
Person Months Worked: 12.00 **Funding Support:**
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National Academy Member: N
Other Collaborators:

Progress Report
Thermodynamically Constrained Averaging
Theory for Multiscale Systems

Cass T. Miller, Principal Investigator
University of North Carolina
23 August 2018

Submission of Publications Under ARO Sponsorship During This Reporting Period

McClure, J.E., A.L. Dye, C.T. Miller, and W.G. Gray (2017) On the Consistency of Scale Among Experiments, Theory, and Simulation, Hydrology and Earth System Sciences Discussions, Vol. 21, pp. 1063--1076, doi:10.5194/hess-21-1063-2017.

Miller, C.T., F.J. Vald\'es-Parada, and B.D. Wood (2017) A Pedagogical Approach to the Thermodynamically Constrained Averaging Theory, Transport in Porous Media, Vol. 119, No. 3, pp. 585--609, doi:10.1007/s11242-017-0900-6.

Anderson, D.M., R.M. McLaughlin, and C.T. Miller (2018) Homogenization of One-Dimensional Draining Through Heterogeneous Porous Media Including Higher-Order Approximations, Physica D, Vol. 365, pp. 42--56, doi: 10.1016/j.physd.2017.10.010.

Miller, C.T., W.G. Gray, and C.E. Kees (2018) Thermodynamically Constrained Averaging Theory: Principles, Model Hierarchies, and Deviation Kinetic Energy Extensions, Entropy, Vol. 20(4), No. 253, doi: 10.3390/e20040253.

Miller, C.T., F.J. Valdes-Parada, S. Ostvar, and B.D. Wood (2018) A Priori Parameter Estimation for the Thermodynamically Constrained Averaging Theory: Species Transport in a Saturated Porous Medium, Transport in Porous Media, Vol. 122, No. 3, pp. 611--632, doi:10.1007/s11242-018-1010-9.

McClure, J.E., R.T. Armstrong, M.A. Berrill, S. Schluter, S. Berg, W.G. Gray, and C.T. Miller (2018) A Geometric State Function for Two-Fluid Flow in Porous Media, in press: Physical Review Fluids.

Weigand, T.M., P.B. Schultz, D.H. Giffin, M.W. Farthing, A. Crockett, C.T. Kelley, W.G. Gray, and C.T. Miller (2018) Modeling Non-Dilute Species Transport Using the Thermodynamically Constrained Averaging Theory, in press: Water Resources Research.

McClure, J.E., Z. Li, A.P. Sheppard, and C.T. Miller (2018) A Volumetric Flux Boundary Condition for Lattice Boltzmann Methods, in review.

Battiato, I., P.T. Ferrero, V.D. O'Malley, C.T. Miller, P.S. Takhar, F.J. Valdes-Parada, and B.D. Wood (2018) Theory and Applications of Macroscale Models in Porous Media, in review.

Miller, C.T., J.E. McClure, and W.G. Gray (2017) Toward the Closure of a New Generation of Multiphase Flow Models, Alliance of Laboratories in Europe for Education, Research and Technology, ALERT Geomaterials Workshop 2017, Aussois, France, 2--4 October 2017.

Miller, C.T. (2017) Coupled Processes and Reactive Transport in Porous Media, Workshop on Excellence in Education and Research: An Adaptive and Integrative Approach for Engineering and Petroleum, King Fahd University of Petroleum and Minerals, Dhahran, Kingdom of Saudi Arabia, 15--17 October 2017.

Bowers, C.A., P.B. Schultz, C.P. Fowler, J.E. McClure, and C.T. Miller (2017) Experimental Observation of Dispersion Phenomenon for Non-Newtonian Flow in Porous Media, Abstract H43I-1766. American Geophysical Union Fall Meeting, New Orleans, Louisiana, 11--15 December 2017.

Bruning, K., S. Kalkowski, and C.T. Miller (2017) Microfluidic Evaluation of the Effects of Wettability on Two-Fluid Flow in Porous Media, Abstract H11G-1284. American Geophysical Union Fall Meeting, New Orleans, Louisiana, 11--15 December 2017.

Fowler, C.P., C.A. Bowers, J.E. McClure, and C.T. Miller (2017) Recent Algorithmic Advances for the Simulation of Porous Medium Systems Using the Lattice Boltzmann Method, Abstract H11G-1285. American Geophysical Union Fall Meeting, New Orleans, Louisiana, 11--15 December 2017.

McClure, J.E., R.T. Armstrong, M.A. Berrill, S. Schluter, S. Berg, W.G. Gray, and C.T. Miller (2017) Digital Rock Physics and Macroscale Models for Two-Fluid Flow, Abstract H11L-05. American Geophysical Union Fall Meeting, New Orleans, Louisiana, 11—15 December 2017.

McClure, J.E., C.L. Talbot, R.T. Armstrong, P. Mostaghimi, Y. Yu, and C.T. Miller (2017) Stochastic Models of Macroscale Quantities for the Prediction of the REV Scale for Multiphase Flow Through Porous Media, Abstract H13A-1348. American Geophysical Union Fall Meeting, New Orleans, Louisiana, 11--15 December 2017.

Miller, C.T., J.E. McClure, and K. Bruning (2017) Lattice-Boltzmann Modeling of Community Challenge Microfluidic Experiments to Evaluate the Effects of Wettability on Two-Fluid Flow in Porous Media, Abstract H14G-04. American Geophysical Union Fall Meeting, New Orleans, Louisiana, 11--15 December 2017.

Talbot, C.L., J.E. McClure, R.T. Armstrong, P. Mostaghimi, Y. Yu, and C.T. Miller (2017) Reduced Dynamic Models of Macroscale Quantities for the Prediction of Equilibrium System States for Multiphase Porous Medium Systems, Abstract H21G-1568. American

Geophysical Union Fall Meeting, New Orleans, Louisiana, 11--15 December 2017.

Valdes-Parada, F.J., S. Ostavar, B.D. Wood, and C.T. Miller (2017) A Predictive Parameter Estimation Approach for the Thermodynamically Constrained Averaging Theory Applied to Diffusion in Porous Media, Abstract H33E-1724. American Geophysical Union Fall Meeting, New Orleans, Louisiana, 11--15 December 2017.

Weigand, T.M., E. Harrison, and C.T. Miller (2017) Evaluation and Validation of a TCAT Model to Describe Non-Dilute Flow and Species Transport in Porous Media, Abstract H11F-1244. American Geophysical Union Fall Meeting, New Orleans, Louisiana, 11—15 December 2017.

McClure, J.E., R.T. Armstrong, M.A. Berrill, S. Schluter, S. Berg, W.G. Gray, and C.T. Miller (2018) New Insights into the Geometric State for Two-Fluid Porous Medium Systems, American Physical Society Meeting, Los Angeles, California, 5--9 March 2018.

Fowler, C.P., C.A. Bowers, J.E. McClure, and C.T. Miller (2018) Simulation of Non-Newtonian Fluid Flow Through Porous Media Using Lattice Boltzmann Methods, Society for Industrial and Applied Mathematics, 42nd Southeastern Atlantic SIAM Conference, Chapel Hill, North Carolina, 9--11 March 2018.

Weigand, T.M., M.Q. de Luna, M.W. Farthing, C.E. Kees, and C.T. Miller (2018) A Fully Second Order Entropy Viscosity Model for Species Transport in Porous Media, Society for Industrial and Applied Mathematics, 42nd Southeastern Atlantic SIAM Conference, Chapel Hill, North Carolina, 9--11 March 2018.

Bruning, K., S. Kalkowski, and C.T. Miller (2018) Microfluidic Evaluation of the Effects of Wettability on Two-Fluid Flow in Porous Media, Abstract 643. International Society for Porous Media, 10th Annual Meeting and Jubilee, New Orleans, Louisiana, 14--17 May 2018.

Fowler, C.P., C.A. Bowers, K. Bruning, J.E. McClure, and C.T. Miller (2018) Advancements in Large-Scale Simulation of Microscale Porous Medium Systems Using Lattice Boltzmann Methods, Computational Methods in Water Resources XXII, Saint Maloes, France, 3--7 June 2018.

Miller, C.T., J.E. McClure, K. Bruning, and W.G. Gray (2018) Toward a New Generation of Two-Fluid-Phase Flow Models: Theory, Computations, Experiments, and Remaining Challenges, Computational Methods in Water Resources XXII, Saint Maloes, France, 3--7 June 2018.

Miller, C.T., J.E. McClure, C.L. Talbot, and W.G. Gray (2018) Bridging Microscale and Macroscale Descriptions of Two-Fluid Flow in Porous Media Using Theoretical and Large-

Scale Computational Approaches, Gordon Research Conference, Flow and Transport in Permeable Media, Newry, Maine, 8--13 July 2018.

Bowers, C.A., P.B. Schultz, and C.T. Miller (2018) Modeling and Experimental Observations of Non-Newtonian Species Dispersion in Porous Medium Systems, Abstract. American Geophysical Union Fall Meeting, Washington, D.C., 10--14 December 2018.

Bruning, K., S. Kalkowski, and C.T. Miller (2018) Microfluidic Evaluation of the Effects of Wettability on Two-Fluid Flow in Porous Media, Abstract. American Geophysical Union Fall Meeting, Washington, D.C., 10--14 December 2018.

Fowler, C.P., J.E. McClure, and C.T. Miller (2018) A Multi-Color Lattice Boltzmann Approach for the Simulation of Three-Fluid Phase Flow Through Porous Medium Systems, Abstract. American Geophysical Union Fall Meeting, Washington, D.C., 10--14 December 2018.

Shepherd, B., W.G. Gray, C.E. Kees, I. Rybak, and C.T. Miller (2018) Modeling Sediment Transport in Three-Phase Surface Water Systems, Abstract. American Geophysical Union Fall Meeting, Washington, D.C., 10--14 December 2018.

Talbot, C.L., C.P. Fowler, and C.T. Miller (2018) Bayesian Models of Scaling and Correlation of Macroscale State Variables in Multiphase Flow Through Porous Media, Abstract. American Geophysical Union Fall Meeting, Washington, D.C., 10--14 December 2018.

Weigand, T.M., and C.T. Miller (2018) Microscale Simulation of Non-Dilute Flow and Transport in Porous Media, Abstract. American Geophysical Union Fall Meeting, Washington, D.C., 10--14 December 2018.

Miller, C.T., and W.G. Gray (2018) Recent Advances in Modeling Multiphase Flow Using the Thermodynamically Constrained Averaging Theory, Workshop on Advanced Computational Modeling for Tumor Growth Prediction, Institute for Advanced Study, Technical University of Munich, Munich Germany, 24--26 September 2018.

Miller, C.T., J.E. McClure, C.P. Fowler, and W.G. Gray (2018) Microscale Simulation of Porous Medium Systems for Closure, Evaluation, and Validation of TCAT Models, US Army Engineer Research and Development Center, Vicksburg, Mississippi, 19 April 2018.

Miller, C.T., A New Generation of Models to Describe Two-Fluid Flow in Porous Medium Systems, Department of Mathematics, University of Padova, Padova, Italy, 27 September 2018.

Miller, C.T., A New Generation of Models to Describe Two-Fluid Flow in Porous Medium Systems, College of Petroleum Engineering and Geosciences, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia, 30 September 2018.

Student/Supported Personnel Metrics for This Reporting Period

This project supported the full-time Ph.D. studies of Mr. Timothy M. Weigand. He is a senior doctoral student expected graduate this calendar year. He collaborates with Matthew Farthing and Chris Kees from the ERDC lab.

Technology Transfer

The PI and his research group maintain active, and productive, collaborations with Dr. Matthew W. Farthing and Dr. Christopher E. Kees, both from the ERDC lab in Vicksburg, Mississippi. Current joint work includes the development of a sediment transport model based upon the thermodynamically constrained averaging theory (TCAT), the evaluation and validation of a TCAT model for non-dilute transport in porous media, and the use of TCAT to formulate and compute the rate of entropy production for use in entropy-viscosity-based numerical approximation methods being developed at ERDC. Publications and presentations document a record of accomplishment along these collaborative lines.

Scientific Progress and Accomplishments

Progress and accomplishments over the previous year include the following specific areas: single-fluid flow and transport, two-fluid flow, three-fluid flow, sediment transport, and entropy viscosity methods.

Single-fluid flow and transport accomplishments fall into two categories: non-dilute species transport and non-Newtonian flow through porous media. Non-dilute species transport work has resulted in presentations and a paper in press that shows that a TCAT model provides an improved representation of observed behavior compared to all previous efforts, which have included a range of phenomenological and formal mathematical approaches, such as homogenization. Non-Newtonian work has focused on modeling the flow of shear-thinning fluids through a porous media and dilute species transport for such flows. Agreement with experimental data is encouraging and a publication detailing this work will be submitted in the near future; a generalization of the results to other media is being considered; a TCAT model to derive closure relations from first principles is being formulated; and a microscale model describing species transport has been implemented and is being compared to experimental data. Several publications should result from this mostly finished work.

Two-fluid flow accomplishments are, we believe, landmark contributions to the field that should greatly influence future applications in many areas of science. The results are technical but can be summarized in an easily digestible form. Two-fluid flow occurs in many areas of science including environmental applications, petroleum recovery, carbon sequestration, soil physics, fluid movement in plants, and many biomedical applications. Mathematical models used to describe fluid flow for these applications were formulated about 50 years ago phenomenologically. Closure relations are time-history dependent, or hysteretic, and variables known to be important at small scales are absent from commonly applied models. A primary goal of this project was to resolve these issues and produce a new class of scale-consistent models; this has been the holy grail in this field for decades. We produced a paper in press in Physical Review Fluids that demonstrates using ideas from topology and extending to porous medium physics that a non-hysteretic state equation exists to describe capillary pressure. We have not only theoretically shown this, but we have also done an extensive set of very large-scale simulations that confirm this finding for a wide range of porous media. One of the consequences of this work is that an evolution equation is needed for the Gaussian curvature at the macroscale to close this new class of model. We have recently derived a candidate equation, which is the final major missing piece of this model. Some other loose ends exist to tie up, but these are relatively straightforward. Several additional papers should result from this work.

Three-fluid flow accomplishments include the extension of our lattice-Boltzmann two-fluid-flow model to three-fluid phases. We have documented good performance on hybrid node supercomputers for this work, and we have performed several validations. This work will enable our continued work in this field in which the models are both extremely difficult and relatively poorly developed. The TCAT theory has not been done on this class of problem yet, but it could be, opening up another broad class of application. We will publish our computational results from this work and have presentations scheduled.

Sediment transport accomplishments include the completion of a manuscript that comprehensively reviews the field, formulates a general class of three-phase models, provides entropy production conditions that all models must satisfy, and analyzes a leading sediment transport model, showing that it can violate the entropy production inequality. This comprehensive work required a substantial, sustained effort, but it provides a foundation for substantial potential future work to formulate, evaluate, and validate a new class of high-fidelity models of interest to ERDC researchers, and many others interested in sediment transport.

Entropy viscosity method accomplishments include formulation of an approach to replace ad hoc formulations of entropy production with first principles, physically based methods of computing entropy production based upon TCAT to add the required dissipation to continuous finite element methods. This can be seen as an alternative to finite volume methods used to approximate hyperbolic conservation equations with the benefit of handling unstructured grids. A manuscript detailing this work will be completed in the near future and presentations of these results are scheduled.

Plans for Next Reporting Period

The funding for this project has been spent out. Thus, no plans are reported for the next year. Of course, publications in the works based upon work already accomplished will be completed. These include a sediment manuscript that will be submitted with the next week, and a publication on TCAT entropy viscosity methods, both in collaboration with ERDC researchers. Several other publications are in the final stages, and we will credit ARO support as applicable.