NATIONAL ENERGY TECHNOLOGY LABORATORY
OIL & GAS

DOE Award No.: FP00008138

Quarterly Research Performance Progress Report
(Period Ending 6/30/2019)

NUMERICAL STUDIES FOR THE CHARACTERIZATION OF RECOVERABLE RESOURCES FROM METHANE HYDRATE DEPOSITS

Project Period (August 1, 2018 to Open)

Submitted by:
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U.S. DEPARTMENT OF ENERGY | NATIONAL ENERGY TECHNOLOGY LABORATORY

Office of Fossil Energy

RESEARCH PERFORMANCE PROGRESS REPORT

DISCLAIMER

ACCOMPLISHMENTS:

Task 1. Project Management Plan

Status: Ongoing

A Draft PMP was submitted for Budget Period #1 in July 2018, with a revised FWP and SOPO.

Task 2. Code Maintenance, Updates, and Support

Status: Ongoing

The three-part paper series documenting the TOUGH+HYDRATE/Millstone suite was published in Q3:

Moridis, G.J., Reagan, M.T., Queiruga, A.F., "Simulation of Gas Production from Multilayered Hydrate-Bearing Media with Fully Coupled Flow, Thermal, Chemical and Geomechanical Processes Using TOUGH+Millstone, Part I: The Hydrate Simulator," *Transport in Porous Media*, **128**, 405-430, doi: 10.1007/s11242-019-01254-6.

Queiruga, A.F., Moridis, G.J., Reagan, M.T., "Simulation of Gas Production from Multilayered Hydrate-Bearing Media with Fully Coupled Flow, Thermal, Chemical and Geomechanical Processes Using TOUGH+Millstone, Part II: Geomechanical Formulation and Numerical Coupling" *Transport in Porous Media*, **128**, 221-241, doi: 10.1007/s11242-019-01242-w.

Reagan, M.T., Queiruga, A.F., Moridis, G.J., “Simulation of Gas Production from Multilayered Hydrate-Bearing Media with Fully Coupled Flow, Thermal, Chemical and Geomechanical Processes Using TOUGH+Millstone, Part III: Application to Production Simulation,” *Transport in Porous Media*, **129**, 179-202, doi: 10.1007/s11242-019-01283-1.

An invited talk concerning the TOUGH+Millstone coupling was presented in Q2:

Task 3. Support of DOE’s Field Activities and Collaborations
Subtask 3.1: Design support for a DOE-led field test in the North Slope of Alaska
Status: Pending

We did not begin discussions about the upcoming field test in Q3. Meetings have been scheduled in Q4, and activities on this task will begin in July 2019.

Subtask 3.2: Activities in support of DOE international gas hydrate collaborations
Status: Ongoing

Our group finished the paper for the JMPG Special Edition on the India Gas Hydrates program, and the paper remains in press pending the completion of the special issue.

Subtask 3.3: Participation in the Code Comparison Study
Status: Ongoing

LBNL contributed solutions to Problems #1, #2, and #4, and designed Problem #3. We participated in regular teleconferences with study leaders and other simulation teams. The insights gained from the CCS have led to the development of a new code testing and validation system for TOUGH+HYDRATE (see Task 2), as well as motivating us to perform addition evaluations of the TOUGH+ code architecture, numerical methods, and other issues.

The Problem #3 formulation and the analysis of the results included a mesh-convergence study for both TOUGH+HYDRATE and the TOUGH+HYDRATE+Millstone flow-geomechanical suite. This is the first such study that we are aware of, and contributes to the understanding of the mesh generation methodologies used to create reservoir models for TOUGH+HYDRATE and other Darcy-based hydrate reservoir simulators. Problem #3 also involved comparison to an analytical solution for the case of 1-D reservoir depressurization with geomechanical response. Iterative testing of the codes (via parametric sensitivity studies) led to a very close match between the analytical and simulated solutions (Figure 1), providing a direct verification/validation experiment for the TOUGH+ codes.

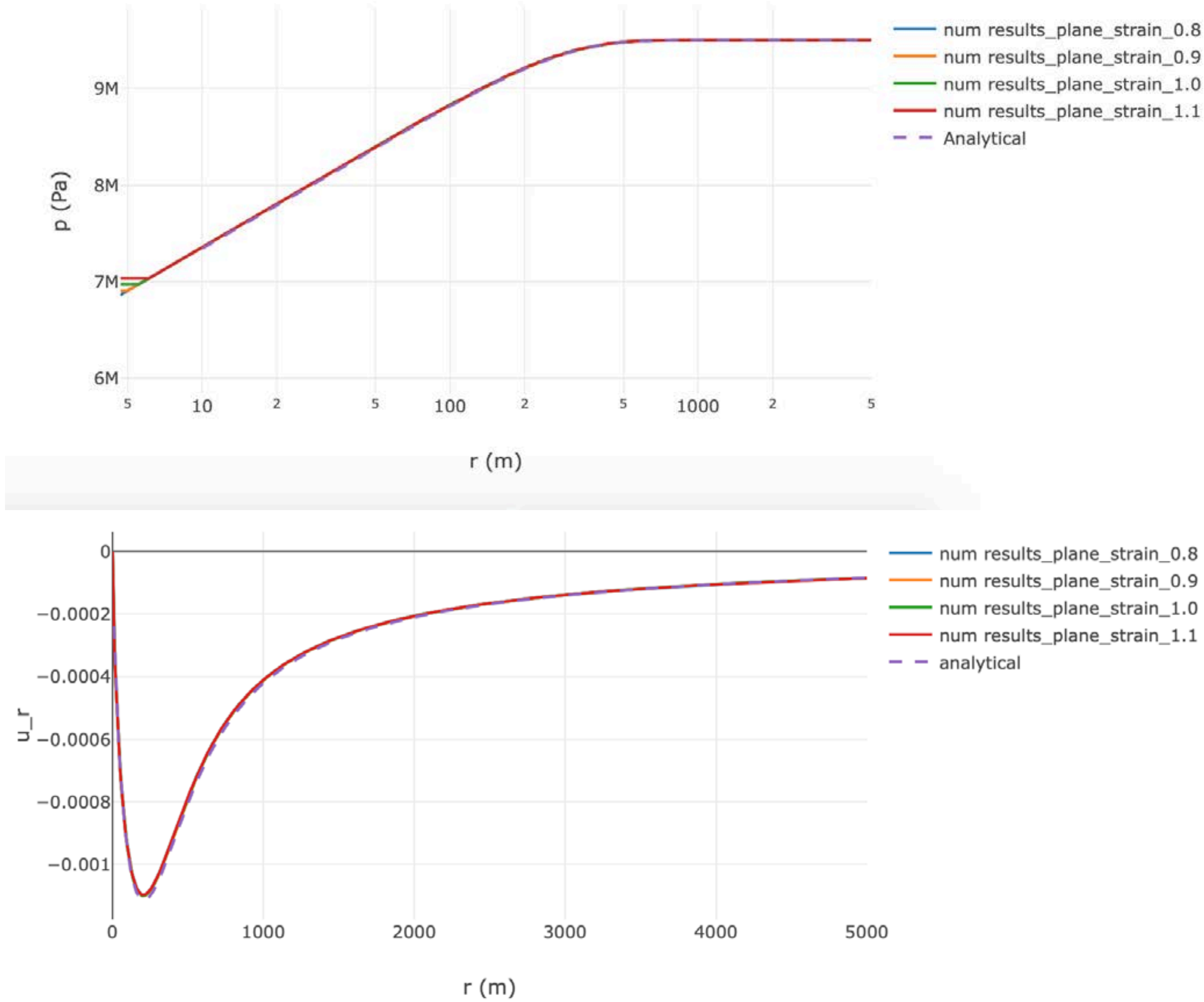

Figure 1: Pressure (top) and radial displacement (bottom) for a 1-D radial system undergoing depressurization. The dotted line represents the analytical solution, the solid line the TOUGH+HYDRATE+Millstone solution.

In Q3, LBNL lead the writeup of Problem 3 for the final IGHCCS2 report and publication(s).

Task 4. Exploration of High-Efficiency Modeling Methods for Hydrate Reservoir Simulation
Status: Ongoing

In this quarter, we have made major progress on the machine learning based approach to solving multiphase, multicomponent reservoir simulation problems. The general direction of this line of work has been demonstrating the use of differentiable programming in scientific and engineering applications.

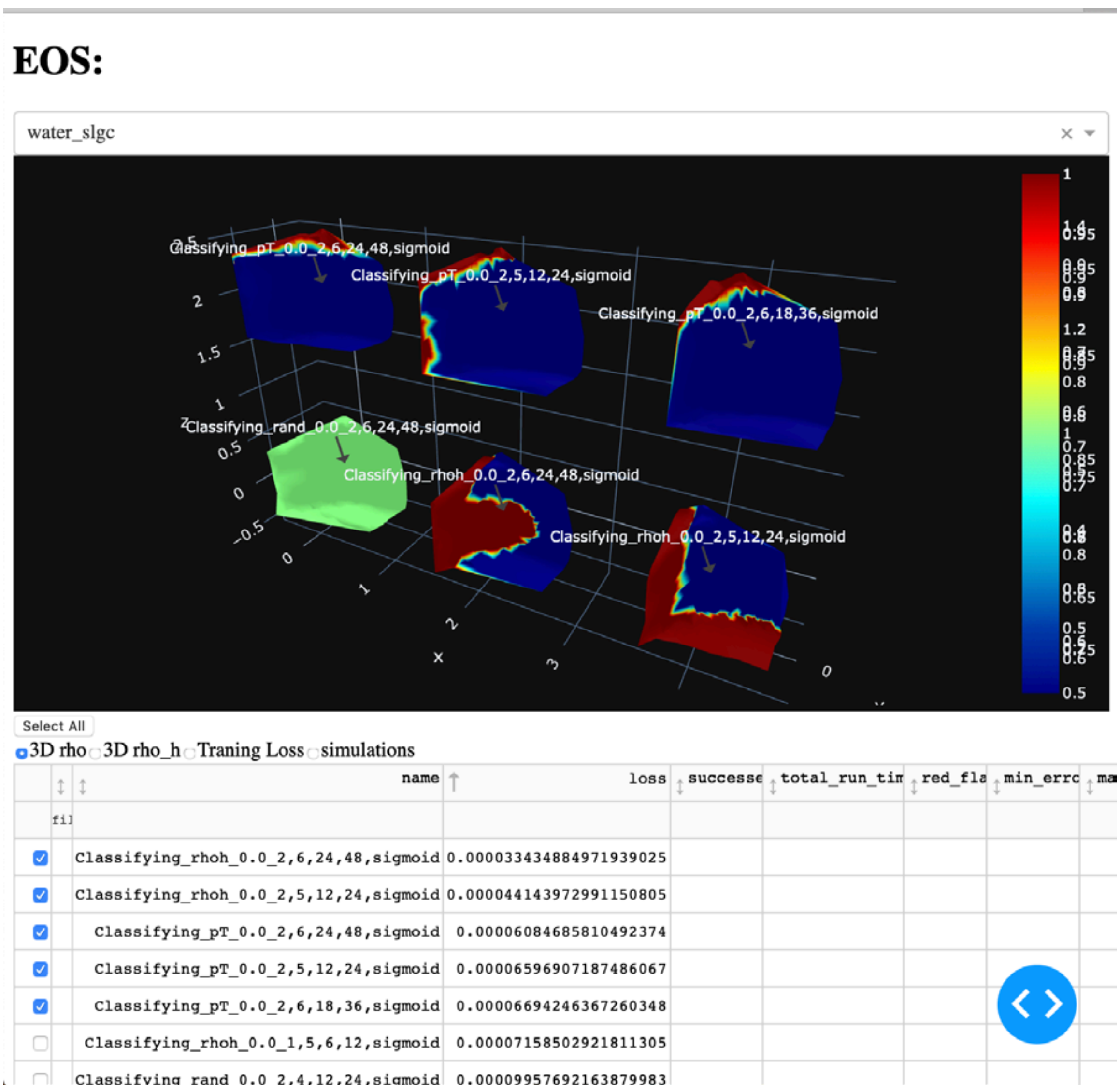

Figure 2: Screen shot of the Dash web interface for examining learning of equation of state representations.

We are replacing the state-machine based specification of phase transitions (the traditional TOUGH “EOS”) with the deep-learning technique of an autoencoder, to learn a new representation of the constraint manifold (the multidimensional, multi-phase space). The original description of the problem, which was solving for a changing set of thermodynamic primary variables, is transformed to solving unknowns on the latent space of the autoencoder. In this quarter, the method has now been demonstrated to be able to solve simulations involving phase changes, using a novel parameterization of phase/mixture enthalpies. To evaluate, visualize, and analyze the success of the method, we have written a custom, Python-based Dash web-based GUI, which is shown in Figure 2. The web application is able to parse the "database" structure of EOS definitions with multiple model checkpoint files to display 3D renderings of the surfaces, plots of test simulations, and training performance alongside a table of each architecture's performance metrics. As seen in the Figure, at the top is a dropdown menu of all EOS definitions in the database (currently set to "water_slgc" for solid-liquid-gas-supercritical). At the bottom of the page is a scrolling list of all model architectures that were trained for this EOS. In the center of the screen is a 3D rendering of the temperature-pressure-density surface for the selected models. The center panel can change to show different 3D renderings, training loss, or simulation results from the testing suite.

This type of GUI will evolve into the tool used by scientists to automatically generate new EOS modules from experimental or other datasets without the need to parameterize “by hand” multiple equations to represent phase boundaries or other EOS properties. We are currently deriving the training dataset for the equilibrium methane-hydrate EOS to extend the method to two-species problems. A manuscript on the method is in preparation, with a focus on the multiphase EOS problem as a generalized constrained differential algebraic equation.

The Python implementation of equations of state for water from literature that was used to assemble the training set are available on GitHub:

https://github.com/afqueiruga/equations_of_state

The prototype codebase is currently in the last stages of validation and debugging, and manuscript preparation has begun with the end goal of preparing the newly developed computational techniques for end-of-budget-period release and usage in a production simulation package.

Task 5. Publications, Tech Transfer, and Travel
Status: Ongoing

No new submitted publications in this quarter.

Conference travel to date:

1. Mastering the Subsurface, Carbon Storage and Oil and Natural Gas Conference, Pittsburgh, PA 13-16 August 2018.
2. Machine Learning in Solid Earth Geoscience, Santa Fe, Nevada, March 2019
3. SIAM Conference on Mathematical & Computational Issues in Geosciences, Houston, Texas, March 2019

Milestone Table

Milestone Title	Milestone Description	Planned Completion Date	Actual Completion Date	Status / Results
PMP	Maintenance and update of the Project Management Plan	August 30, 2018	Included with SOPO 7/25/18	Submitted
Deliverable	Updated versions serial and parallel versions of the T+H/Millstone code	May 30, 2019	April, 2019	Three-paper series describing software published in TiPM.
Deliverable	Report describing the design and performance of the proposed field test.	August 31, 2019		Simulations of the field test delayed pending disclosure of data.
Deliverable	Completion participation in the code comparison study; contributions to reports and publications	August 31, 2019		
Deliverable	An assessment of the feasibility, effectiveness and robustness of ROMs	August 31, 2019		

PRODUCTS:

Publications to date (this BP):

1. Moridis, G.J., Reagan, M.T., Queiruga, A.F., "Simulation of Gas Production from Multilayered Hydrate-Bearing Media with Fully Coupled Flow, Thermal, Chemical and Geomechanical Processes Using TOUGH+Millstone, Part I: The Hydrate Simulator," *Transport in Porous Media*, **128**, 405-430, doi: 10.1007/s11242-019-01254-6.
2. Queiruga, A.F., Moridis, G.J., Reagan, M.T., "Simulation of Gas Production from Multilayered Hydrate-Bearing Media with Fully Coupled Flow, Thermal, Chemical and Geomechanical Processes Using TOUGH+Millstone, Part II: Geomechanical Formulation and Numerical Coupling" *Transport in Porous Media*, **128**, 221-241, doi: 10.1007/s11242-019-01242-w.
3. Reagan, M.T., Queiruga, A.F., Moridis, G.J., "Simulation of Gas Production from Multilayered Hydrate-Bearing Media with Fully Coupled Flow, Thermal, Chemical and Geomechanical Processes Using TOUGH+Millstone, Part III: Application to Production Simulation," *Transport in Porous Media*, **129**, 179-202, doi: 10.1007/s11242-019-01283-1.
4. Moridis, G.J., Reagan, M.T., Queiruga, A.F., Collett, T.S., Boswell, R., Evaluation of the Performance of the Oceanic Hydrate Accumulation at the NGHP-02-9 Site of the Krishna-Godavari Basin During a Production Test and Under Full Production, *J. Marine and Petroleum Geology,* in press, doi: 10.1016/j.marpetgeo.2018.12.001.
5. Moridis, G.J., Reagan, M.T., Queiruga, A.F., Kim, S.J., System response to gas production from a heterogeneous hydrate accumulation at the UBGH2-6 site of the Ulleung basin in the Korean East Sea, *J. Pet. Sci. Eng.,* **178**, 655-665. doi: 10.1016/j.petrol.2019.03.058.

Presentations to date (this BP):

1. “Numerical Studies for the Characterization of Recoverable Resources from Methane Hydrate Deposits,” Mastering the Subsurface, Carbon Storage and Oil and Natural Gas Conference, Pittsburgh, PA 13-16 August 2018.
2. “Numerical Studies for the Characterization of Recoverable Resources from Methane Hydrate Deposits,” project wrapup meeting. 28 September 2018.
3. "Machine Determination of Better Representations of Multiphase Equation of States for Subsurface Flow Simulation" at Machine Learning in Solid Earth Geosciences, 18-22 March 2019 in Santa Fe, NM.
4. “Fully Coupled Multimesh Algorithms for Nonisothermal Multiphase Flow and Mechanics in Geological Formations,” **(invited)** SIAM Conference on Mathematical & Computational Issues in Geosciences, Houston, Texas, March 2019.

SPECIAL REPORTING REQUIREMENTS:

N/A

BUDGETARY INFORMATION:

Actual Cost (this quarter)	Actual Cost (cumulative for BP)	Funds available (for the BP)	Balance of unspent funds (for the BP)	Actual Cost (cumulative for the full FWP)	Funds available (for the full FWP)	Balance of unspent funds (for the full FWP)
$63,063	$318,015	$500,000	$181,985	$318,015	$500,000	$181,985

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