NATIONAL ENERGY TECHNOLOGY LABORATORY
OIL & GAS

DOE Award No.: FP00008138

Quarterly Research Performance Progress Report

(Period Ending 12/31/2018)

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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Signature

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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

In Q4, debugging of the TOUGH+HYDRATE/Millstone combination continued. Inspired by discussions in the IGHCCS2 meetings, we developed a new set of test problems for T+H. These test problems are designed to auto-run after code compilation, automatically testing whether code upgrades or modifications affect the validity of the code and results. In addition, we performed additional convergence testing, to establish a formal baseline for mesh discretization decisions.

The results were reported to the IGHCCS2 group to inform other teams' code development and testing strategies.

In additional, the three-part paper series documenting the TOUGH+HYDRATE/Millstone suite went through a second round of revisions:

Moridis, G.J., Reagan, M.T., Queiruga, A.F., “The TOUGH+Millstone Code for the Analysis of Coupled Flow, Thermal, Chemical and Geomechanical Processes in Hydrate-Bearing Geologic Media, Part I: The Hydrate Simulator,” submitted to *Transport in Porous Media*.

Queiruga, A.F., Moridis, G.J., Reagan, M.T., “The TOUGH+Millstone Code for the Analysis of Coupled Flow, Thermal, Chemical and Geomechanical Processes in Hydrate-Bearing Geologic Media, Part II: Numerical Algorithms and the Stone Geomechanical Simulator,” *Transport in Porous Media*, in press.

Reagan, M.T., Queiruga, A.F., Moridis, G.J., “The TOUGH+Millstone Code for the Analysis of Coupled Flow, Thermal, Chemical and Geomechanical Processes in Hydrate-Bearing Geologic Media, Part III: Application to Production Simulation,” submitted to *Transport in Porous Media*.

Part II has been accepted for publication. Parts I and III are in a final round of review.

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 have not begun discussions about the upcoming field test.

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

Status: Ongoing

Our group finished the third revision on the paper to be published in the JMPG Special Edition on the India Gas Hydrates program. The revision involved new scoping simulations to clarify reviewer comments and update results and figures.

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.

A paper related to the DOE collaboration with KIGAM was accepted for publication:

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.

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).

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

Status: Ongoing

Using the lens of machine learning, we have reformulated the problem of multiphase flow and are developing a new algorithm to both implement and program the simulations. We use deep learning techniques to learn new representations of the complex equations of state that can be directly employed inside of a mass-and-energy balance formulation.

The biggest challenge in simulation of subsurface flows is the representation of complex multiphase and multicomponent fluids and solids. The phase-change logic is a bottleneck to simulation performance due to the complex hydrate phase behavior. The equation of state is usually treated as sets of empirical fits broken up according to specific phase combinations, derived by scientists according to their knowledge of multiphase thermodynamics. The descriptions become combinatorially more complex as species and phases are added, resulting in combinatorially more human labor and combinatorially more code and more branching logic.

This new technique treats the equation of state as a local point-wise manifold constraint on the intensive material fields, to be coupled with the balances of momentum and energy. The constraint surface is represented as a database of coordinates in high-dimensional density-enthalpy-pressure-temperature-etc. space. A new representation of primary variables is learned by training an autoencoder on the thermodynamic dataset. The optimized model is then plugged into the balance equations, generating the system of differential algebraic equations that are a function of the discovered primary variables.

We have demonstrated that the deep learning algorithm is able to perform unsupervised identification of distinct phases in the equation of state. The approach of employing deep learning on constraint representations has been validated on the classical pendulum, the most basic constrained differential equation. The methodology and corresponding software system for training and simulation for multiphase properties is under development. The validation dataset is a pure water equation of state spanning the liquid-gas-ice-supercritical regimes. The training system is implemented in Google's TensorFlow package. A single grid-block prototype simulation has been written to solve the new formulation.

This first prototype will be presented at an invited talk:

"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.

After demonstrating effective simulations on the pure-water equation of state, the next steps will apply this machine-learning algorithm to a methane hydrate dataset. The system will then be extended to use machine learning to build more efficient models for other properties in a flow simulation.

Task 5. Publications, Tech Transfer, and Travel

Status: Ongoing

No travel or submitted publications in the first five months of the Budget Period.

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		
Deliverable	Report describing the design and performance of the proposed field test.	August 31, 2019		
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):

n/a

Presentations to date (this BP):

“Numerical Studies for the Characterization of Recoverable Resources from Methane Hydrate Deposits,” project wrap-up meeting. 28 September 2018.

“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.

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)
$105,974	$189,497	$500,000	$310,503	$189,497	$500,000	$310,503

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