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Quarterly Research Performance Progress Report

(Period Ending 03/31/2018)

Kinetic Parameters for the Exchange of Hydrate Formers

Project Period (07/01/2013 to open)

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NATIONAL ENERGY TECHNOLOGY LABORATORY

Office of Fossil Energy

RESEARCH PERFORMANCE PROGRESS REPORT

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ACCOMPLISHMENTS:

BP5-Task 13.0 Nitrogen Injection (KIGAM-funded, Separate, Coordinated PNNL Project #68908)

An interim report, entitled "Numerical assessment of natural gas hydrate production via nitrogen injection," was submitted to the KIGAM client that documented a series of numerical simulations executed with STOMP-HYDT-KE code, against a series of experiments conducted by the Dalian University and Zhejiang University (Zhang et al., 2017). These experiments considered the injection of nitrogen into a hydrate bearing column of glass beads. The experiments were split into two cases; one that varied the nitrogen flow rate through the column and one that varied the initial hydrate saturation. Temperatures and pressures within the experimental column were maintained within the hydrate stability region for pure methane hydrate, which made this experiment an appropriate choice for testing the ability of STOMP-HYDT-KE to model hydrate dissociation with the injection of nitrogen. A series of simulations were conducted against the first three experimental cases that varied nitrogen flow rates. For each experimental case, the hydrate dissociation kinetic parameter and guest-molecule kinetic parameter were adjusted to great a reasonable match with the experimental results.

The ability of the STOMP-HYDT-KE simulator to model the dissociation of methane hydrate in a sediment via nitrogen injection was confirmed by modeling the experiments of Zhang et al. (2017). The STOMP-HYDT-KE model for driving hydrate dissociation or formation, based on the mobile phase partial pressures and hydrate equilibrium pressures allows for good agreement with the experimental observations. Two aspects of the comparisons need to be investigated further: 1) decay in hydrate dissociation rates with small hydrate saturations, and 2) the incomplete dissociation of hydrate for the higher initial hydrate saturation scenario. To resolve these issues, additional experimental papers will be investigated that address hydrate dissociation with either nitrogen or air injection.

Zhang, L., Y. Kuang, X. Zhang, Y. Song, Y. Liu, and J. Zhao. 2017. "Analyzing the Process of Gas Production from Methane Hydrate via Nitrogen Injection." Ind. Eng. Chem. Res., 56:7585-7592.

BP5-Task 14.0 Geomechanics Implementation and Verification

This task is closely linked with the BP5-Task 13.0 and 15.0, as geomechanical modeling capabilities are required to complete the nitrogen injection simulations and the code comparison study problems. Accomplishments reported for BP5-Task 13.0 and 15.0 equally during this quarter equally apply to this task.

BP5-Task 15.0 International Hydrate Code Comparison

The 2nd International Gas Hydrate Code Comparison Study progressed through a series of code overviews to the development and solution of a series of four benchmark problems. The series of code overviews were designed to give each participating team an opportunity to describe their computer code(s), but also to acquaint the participants with each other. During this quarter a series of four benchmark problems were identified, along with problem champions: 1) Hydrate dissociation in a radial domain (Mark White, PNNL, USA); 2) Extended Terzaghi Problem (Shubhangi Gupta, GEOMAR Kiel, Germany); 3) Radial domain with coupled flow and geomechanics (Matt Reagan, Alejandro Queiruga, and George Moridis, LBNL, USA); and 4) Nankai Trough (Sayuri Kimoto, Kyoto University, Japan). The study currently comprises 54 participants, representing 24 teams, from 5 countries (i.e., United States, United Kingdom, Germany, Korea, Japan, and China). A workspace within the NETL EDX system has been created for the study, and accounts have been granted for requesting participants. Six study teleconferences were held during the quarter:

- Teleconference #3: January 11, 2018
 - A THCM Code for Methane Hydrate Reservoirs Numerical Implementation and Benchmarks, Shubhangi Gupta (GEOMAR Kiel, Germany)
 - CODE_BRIGHT-HYDRATE Code Description Overview, Marcelo Sánchez (Texas A&M University, USA)
 - o Coupled Hydromechanical Benchmark Problem, Mark White (PNNL, USA)
- Teleconference #4: January 25, 2018
 - o COMVI-MH Code Description Overview, Sayuri Kimoto (Kyoto University, Japan)
 - UC Berkeley THM Code and Constitutive Models Description Overview, Kenichi Soga (UC Berkeley, USA)
 - o STOMP-HYDT-KE Code Description Overview, Mark White (PNNL, USA)
- Teleconference #5: February 08, 2018
 - NETL-Pitt Hydrate Simulator Code Description Overview, Jeen-Shang Lin (University of Pittsburgh, USA)
 - K-Hydrate Simulator Code Description Overview, Jung-Tae Kim (KAIST, Korea)
 - Geo-COUS Simulator Code Description Overview, Hosung Shin (University of Ulsan, Korea)
- Teleconference #6: February 22, 2018
 - o IGHCCS2 Benchmark Problem #1 Description, Mark White (PNNL, USA)
 - IGHCCS2 Benchmark Problem #2 Description, Shubhangi Gupta (GEOMAR Kiel, Germany)
- Teleconference #7: March 08, 2018
 - IGHCCS2 Benchmark Problem #1 Scheduling and Problem Submission Questions, Mark White (PNNL, USA)
 - IGHCCS2 Benchmark Problem #2 Possible Problem Settings and Scheduling, Shubhangi Gupta (GEOMAR Kiel, Germany)

- Teleconference #8: March 22, 2018
 - IGHCCS2 Benchmark Problem #3 Problem Description and Discussions, Matt Reagan and Alejandro Queiruga (LBNL, USA)

The study teleconferences were principally focused on code descriptions and establishing initial benchmark problems. All teleconferences were recorded and those recordings were posted on the NETL EDX system, along with the slide decks from the presentations. A logo for the study was created based on the infamous burning gas hydrate photo taken by Bill Lawson.

MILESTONES:

Milestone Title	Milestone Description	Planned Completion Date	Actual Completion Date	Status / Results
Nitrogen Injection (KIGAM- funded, Separate, Coordinated PNNL Project #68908)	Conduct a series of numerical simulations using its STOMP-HYDT-KE simulator to assess the feasibility of the nitrogen injection technology for production natural gas.	6/30/2018		Simulations with STOMP- HYDT-KE against a series of nitrogen injection experiments. Dr. Won Suk Lee visiting PNNL during April to discuss next steps.
Geomechanics Implementation and Verification	Develop algorithms for its STOMP- HYDT-KE simulator for computing the geomechanical properties as a function of hydrate saturation.	3/31/2018	3/31/2018	Verification simulation executed with STOMP- HYDT-KE against the classical Terzaghi problems.
IGHCCS2: Problem Definition	Initial Problem Set Drafted and Participants Identified for the 2nd International Hydrate Code Comparison Study.	9/30/2017	09/30/2017	A series of four benchmark problems have been identified along with problem champions. Problem descriptions being developed and vetted.
IGHCCS2: Problem Issue	Initial Problem Set Issued for the 2nd International Hydrate Code Comparison Study.	12/31/2017	12/31/2017	Problem #1 released, and first solution submissions reviewed on April 12, 2018 during the IGHCCS2 teleconference.
IGHCCS2: Problem Submission	Initial Problem Set Submission for the 2nd International Hydrate Code Comparison Study.	6/30/2018	4/12/2018	Problem #1 released, and first solution submissions reviewed on April 12, 2018 during the IGHCCS2 teleconference.

PRODUCTS:

No publications nor presentations were released this quarter.

IMPACT:

No significant impacts occurred this quarter.

CHANGES/PROBLEMS:

The IGHCCS2 is progressing with benchmark problems being developed and submissions being review. Participants are joining the regularly scheduled teleconferences, but discussions are minimal.

SPECIAL REPORTING REQUIREMENTS:

No special reporting requirements occurred during this quarter.

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)
\$12,594	\$25,090	\$100,000	\$74,910	\$262,110	\$370,000	\$107,890

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