Research Performance Progress Report

SUBMITTED TO

U. S. Department of Energy
National Energy Technology Laboratory

WORK PERFORMED UNDER AGREEMENT

DE-FE0013919

Project title: Mechanisms for Methane Transport and Hydrate Accumulation in Coarse-Grained Reservoirs

SUBMITTED BY
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October 27, 2015

DUNS number: 1702302390000

RECIPIENT ORGANIZATION
University of Texas at Austin
200 E Dean Keeton St., Stop C0300
Austin, TX 78712-1585

PROJECT PERIOD: October 1, 2013 – September 30, 2017

REPORTING PERIOD END DATE: September 30, 2015

REPORT FREQUENCY: Quarterly

Signed:

Hugh Daigle
ACCOMPLISHMENTS

The project goal is to show, through numerical modeling, how the transport of methane, and the mechanism by which it is transported, control the development of persistent, massive hydrate accumulations in deep sediments below the seabed. The models will be based on recently collected data from Walker Ridge Block 313 (WR 313) in the northern Gulf of Mexico (Figure 1). To achieve the project goal, the project has been divided into three phases. Phase 1 of the project will focus on modifying an existing reservoir simulator (Sun and Mohanty, 2006) to include microbial methane production, salt mass balance and effects on methane stability, and sedimentation. Additional 1-D modeling will provide constraints on expected rates of methanogenesis. Phase 2 of the project will focus on simulations of dissolved methane migration mechanisms to determine if sufficient flux is available to develop the massive hydrate accumulations observed at WR 313. Phase 3 of the project will focus on simulations of free methane gas migration and recycling of methane in the gas phase as it is buried below the base of the methane hydrate stability zone.

The objectives of this project are to define:

1. The dissolved methane flux, organic matter abundance, and time required to develop the accumulations observed at WR 313 by short-distance migration of microbial methane into adjacent coarser-grained layers;
2. The dissolved methane flux and time required to develop the accumulations observed at WR 313 by long-distance, updip migration;
3. Whether there is enough methane in the dissolved phase in the fine-grained sediments to form the observed hydrate deposits or whether a gas phase is present, and if so what the conditions are for three-phase equilibrium;
4. The fate of hydrate that subsides beneath the base of the MHSZ and accumulates as gas, and overpressure generation associated with gas accumulation.

Tasks to be performed
PHASE 1 / BUDGET PERIOD 1
Task 1 - Project management and planning

The Recipient shall work together with the DOE project officer upon award to develop a project management plan (PMP). The PMP shall be submitted within 30 days of the award. The DOE Project Officer shall have 20 calendar days from receipt of the PMP to review and provide comments to the Recipient. Within 15 calendar days after receipt of the DOE's comments, the Recipient shall submit a final PMP to the DOE Project Officer for review and approval.

The Recipient shall review, update, and amend the PMP (as requested by the DOE Project Officer) at key points in the project, notably at each go/no-go decision point and upon schedule
variances of more than 3 months and cost variances of more than 10%, which require amendments to the agreement and constitutes a re-base lining of the project.

The PMP shall define the approach to management of the project and include information relative to project risk, timelines, milestones, funding and cost plans, and decision-point success criteria. The Recipient shall execute the project in accordance with the approved PMP covering the entire project period. The Recipient shall manage and control project activities in accordance with their established processes and procedures to ensure subtasks and tasks are completed within schedule and budget constraints defined by the PMP. This includes tracking and reporting progress and project risks to DOE and other stakeholders.

Task 2 – Reservoir Model Development

The Recipient shall modify an existing general purpose reservoir simulator to include sedimentation, microbial methane production and effect of salt on hydrate equilibrium. The methane equilibrium calculation shall be modified to include changes in water activity due to dissolved salt following the method of Handa (1990). The mass conservation calculation shall be modified to include sedimentation, burial, and changes in porosity over time following the method of Bhatnagar et al. (2007). The initial conditions shall be modified to allow specification of heterogeneous properties (e.g., porosity) throughout the model domain. The boundary conditions shall be modified to allow specification of seafloor sedimentation rate and fluid flux. The Recipient shall verify code modifications with benchmark comparisons of performance with published simulation results (e.g., Bhatnagar et al., 2007).

Task 3 – 1-D Modeling of Microbial Methanogenesis

Concurrently with Task 2, the Recipient shall start with a 1-D reaction-transport model that will follow the burial by sedimentation of a sand layer surrounded by fine-grained sediments. The time-dependent modeling shall track the evolution of gas hydrate formation in the sand layer and shall provide more accurate estimates of the time scales and of the gas hydrate quantities associated with short migration. The methane hydrate stability conditions shall include the effect of pore size in the sand and fine-grained layers following the method of Malinverno (2010). The rate and spatial distribution of microbial methanogenesis shall be constrained by data from scientific ocean drilling expeditions (DSDP, ODP, IODP). The results of this task shall provide first-order constraints on rates of methanogenesis which shall be used as inputs to subsequent tasks (4.1, 4.3, 5.1, 5.2).

PHASE 2 / BUDGET PERIOD 2
Task 4.1 – Short Migration of Dissolved Methane
The Recipient shall investigate short migration of dissolved methane, in which methane generated in fine-grained sediments within the MHSZ is transported by diffusion into adjacent coarse-grained layers in which it forms concentrated hydrate deposits. The simulator developed in Task 2 shall be used for this task. The model domain shall consist of dipping sand layers surrounded by fine-grained sediments. This domain shall be designed to approximate the geometries observed at WR313 with sediment physical properties defined from logs or analog data. Rates of microbial methanogenesis and fluid flow shall be altered to determine the effect each has on the resulting hydrate distribution and time required for accumulation. The model results shall be used to determine the time scale of short migration at WR313, and the distribution of hydrate resulting from short migration.

Task 4.2 – Long Migration of Dissolved Methane

The Recipient shall investigate long migration of dissolved methane, in which dissolved methane is transported by advection from a distant source to the MHSZ. The investigation shall use the simulator developed in Task 2. The model domain shall consist of dipping sand layers surrounded by fine-grained sediments, and shall be designed to approximate the geometries observed at WR313. The model shall assume no local methane generation in the MHSZ and pore water entering the MHSZ with a methane concentration equal to the local solubility. Fluid flux shall be determined assuming that fluid flow is driven by overpressures due to high sedimentation rates (Gordon and Flemings, 1998). The Recipient shall explore the time scale associated with long migration by determining how long is required for fluid flow to form hydrate deposits comparable to those observed at WR313. The Recipient shall additionally simulate situations in which active fluid flow ceases after some time, and investigate how the hydrate that is formed evolves after cessation of fluid flow.

Task 4.3 – Assessment of Flux Associated with Dissolved Methane Migration

The Recipient shall use the model results from Tasks 4.1 and 4.2 to assess the methane flux associated with methane migration in the dissolved phase by either long or short migration. The different scenarios modeled in Tasks 4.1 and 4.2 shall be analyzed to determine methane flux from each migration mechanism, and the time scales and hydrate volumes produced by each. The analysis results shall be compared to the observed hydrate accumulations at WR313 and the age of the host sediments to determine whether migration of dissolved methane could have produced the observed hydrate accumulations.

PHASE 3 / BUDGET PERIOD 3
Task 5.1 – Assessment of Methane Budget Required for Presence of Gas Phase
The Recipient shall use the results of Tasks 4.1 and 4.2 to define methane availability from local, microbial sources as well as deeper sources (thermogenic or microbial). The phase equilibrium implemented in the 3-D model in Task 2 shall be used to determine local solubility within the model domain and determine the amount of methane that may be present as a gas phase. The results of this task will be used to place limits on gas availability in Tasks 5.2 and 5.3.

**Task 5.2 – Free Gas Migration**

The Recipient shall apply a previously established model of hydrate formation (multiphase-flow-controlled, nonequilibrium, neglecting transport of salinity and latent heat) to assess whether the gas phase accumulated beneath the MHSZ can contribute significantly to hydrate saturations within the MHSZ. The Recipient shall evaluate the conditions under which the accumulated gas phase drains into coarse-grained sediment. Having identified those conditions, the Recipient shall evaluate the geologic setting (dip angle, petrophysical properties and multiphase flow properties of the sediment) for which significant updip migration of the gas phase can be expected. The Recipient shall apply the hydrate formation model to geologic settings with significant expected migration to determine the hydrate saturation distribution in the updip direction. The model shall be tested for ranges of the two competing rates (namely, rate of gas accumulation at base of MHSZ and rate of hydrate formation from gas phase and water phase in the MHSZ). The Recipient shall additionally determine the pressure, temperature, and salinity conditions that will permit short migration of a gas phase within the MHSZ. The predicted saturation distributions shall be compared to observations (magnitude of hydrate saturation and its lateral extent) within coarse-grained layers at WR313. If hydrate is predicted to form in the same location and same volume as the accumulations observed at WR313, the Recipient shall determine whether the conditions that give agreement are geologically plausible, and the Recipient shall compare the flux of methane in the gas phase to the fluxes of methane by other mechanisms to be determined in Tasks 4.1 and 4.2. If the rates of methane delivery and time scale of hydrate accumulation are consistent with the accumulations observed at WR313, the Recipient shall use the results to guide the inclusion of free-gas migration phenomena into the full-physics 3D simulations of Task 5.3.

**Task 5.3 – Methane Recycling at the Base of the MHSZ**

The Recipient shall use the reservoir model developed in Task 2 to evaluate the fate of hydrate that moves below the base of the MHSZ as a result of sedimentation. In particular, the Recipient shall examine subsidence of dipping, hydrate-bearing sands of the type encountered at WR313. The Recipient shall model burial of a dipping sand layer through the base of the MHSZ in 3 dimensions. The Recipient shall test different scenarios of sedimentation rate, hydrate saturation in sand layers, and deep methane flux to evaluate gas accumulation below the MHSZ, supply of methane to the base of the MHSZ, and overpressure generated by the accumulation of a
connected gas column. The gas column will be considered connected when it overcomes a percolation threshold of roughly 10% of the pore volume (England et al., 1987). Gas phase pressure shall be computed from gas column height and estimates of capillary pressure from analog sediments (e.g., Blake Ridge; Clennell et al., 1999). The potential to fracture overlying sediments shall be investigated by comparing the resulting pore pressure to the total vertical stress and the minimum horizontal stress.

**Milestone Status Report**

1.A Title: PMP submission  
Planned Date: 4 December 2013  
Completed Date: 22 November 2013  
Verification Method: Submission of final Project Management Plan to DOE within 65 days of start of project.

1.B Title: Project kick-off meeting  
Planned Date: 29 December 2013  
Completed Date: 7 November 2013  
Verification Method: Meeting held within 90 days of start of project.

1.C Title: Sedimentation, microbial methane production, salinity effect implementation  
Planned Date: 30 June 2014  
Completed Date: 30 June 2014  
Verification Method: Implementation of sedimentation, microbial methane production, salinity effect on hydrate stability in 3-D model.

1.D Title: Benchmarking of numerical model against published results  
Planned Date: 31 March 2015  
Completed Date: 31 March 2015  
Verification Method: Simulation results match those obtained from other simulators in 1-D and 2-D (e.g., Bhatnagar et al., 2007; Chatterjee et al., 2011) within 1% in time andhydrate saturation using the same input parameters.

1.E Title: Development of time and methanogenesis constraints for future modeling  
Planned Date: 31 March 2015  
Completed Date: 31 March 2015  
Verification Method: Development of a model that includes time-dependent changes in methane stability in a dipping, subsiding sand layer but matches the results of Cook and Malinverno (2013) for steady-state conditions.
2.A Title: Completion of short migration modeling  
Planned Date: 30 September 2016  
Verification Method: Completion of simulations to evaluate conditions necessary for development of massive hydrate deposits by short migration.

2.B Title: Completion of long migration modeling  
Planned Date: 30 September 2016  
Verification Method: Completion of simulations to evaluate conditions necessary for development of massive hydrate accumulations by long migration.

2.C Title: Quantification of methane flux in the dissolved phase  
Planned Date: 30 September 2016  
Verification Method: Quantification of methane flux associated with methane migration in the dissolved phase by either long or short migration and comparison with existing estimates of methane flux in the northern Gulf of Mexico such as those presented in Frye (2008).

3.A Title: Quantification of methane availability and expected quantities of gas  
Planned Date: 30 September 2017  
Verification Method: Quantification of amount of methane required to form a free gas phase and comparison with existing estimates of methane flux in the northern Gulf of Mexico such as those presented in Frye (2008).

3.B Title: Completion of free gas migration models  
Planned Date: 30 September 2017  
Verification Method: Determinations of methane flux and time necessary to reproduce observed hydrate accumulations at WR313 by migration of free gas.

3.C Title: Completion of modeling efforts to assess methane recycling  
Planned Date: 30 September 2017  
Verification Method: Completion of simulations to assess rates of gas accumulation beneath MSHZ and effect on gas migration and overpressure generation.

What was accomplished under these goals?

Major activities

Task 4.1. Using log data from boreholes WR313-G and WR313-H, we determined the porosity and permeability of the sediments in the methane hydrate stability zone at Walker Ridge. The porosity values were taken from the logs and corrected for the presence of hydrate and poor
borehole conditions. We determined permeability from the corrected porosity and the fraction of clay-sized grains, which we computed from the gamma ray logs. The permeability computation followed the effective medium model recently published by Daigle and Screaton (2015):

\[
(1 - f_c) \frac{k_s - k_c}{k_s + [f_c/(1 - f_c)]k_c} + f_c \frac{k_c - k_e}{k_c + [f_c/(1 - f_c)]k_c} = 0,
\]

(Eq. 1)

where \(f_c\) is the mass fraction of clay-sized grains, \(k_s\) and \(k_c\) are the endmember permeabilities of the (silt+sand)-sized fraction and clay-sized fraction, respectively, and \(k_e\) is the permeability of the sediment. The endmember permeabilities were determined at the corrected in situ porosity value using permeability-porosity relationships determined for Wilcox sandstone (Dutton and Loucks, 2014) and smectite-silica mixtures (Daigle, 2011). Clay-sized fraction \(f_c\) was determined from gamma ray logs using a relationship derived from boreholes in the Mississippi Canyon and Keathley Canyon areas. We verified Eq. 1 by comparing predicted permeabilities with measured permeabilities in the Mississippi Canyon and Keathley Canyon boreholes and found that the predicted values matched the measured values well (Fig. 1) with a 95% confidence interval of 0.62 orders of magnitude.

![Figure 1. Model verification showing predicted versus measured permeability values for U1322 and U1324 (boreholes in Mississippi Canyon) and KC151 (borehole in Keathley Canyon). Solid line is 1:1 correspondence; dashed lines are two standard deviations (±0.62 orders of magnitude).](image-url)
The computed permeabilities at WR313-G and WR313-H are shown in Figs. 2 and 3. The sands in both cases have permeabilities on the order of $10^{-13}$-$10^{-12}$ m$^2$ (roughly 100-1000 millidarcies), while the clays have permeabilities generally $10^{-18}$-$10^{-17}$ m$^2$ (roughly 0.001-0.01 millidarcies). This provides important constraints on the rates of fluid advection at these two locations.

Figure 2. Calculation results for WR313-G. Left to right: clay-sized fraction ($f_c$), porosity, permeability.

Figure 3. Calculation results for WR313-H. Left to right: clay-sized fraction ($f_c$), porosity, permeability.
Based on simple calculation assuming that Poiseuille’s law describes the permeability ($k \propto r^2$, where $r$ is the pore radius), the pore size contrast between the sands and clays at Walker Ridge is on the order of 100-300. Assuming a clay pore size of 100 nm, which is reasonable for marine clays (e.g., Henry et al., 1999; Liu and Flemings, 2011; Day-Stirrat et al., 2012; Daigle and Dugan, 2014), the permeability contrast implies that $r = 30 \mu m$ in sands. This provides important information for solubility calculations.

Using the sediment physical properties we derived from the logs, we modeled accumulation of hydrate in a dipping sand layer through diffusion of microbial methane alone. The sand layer geometry was modeled after the Orange sand at WR313. We assumed that the organic matter concentration at the seafloor was 0.5 wt%, that the methanogenesis rate was $10^{-13}$ s$^{-1}$ (Malinverno, 2010), and that the sedimentation rate was 1 mm/yr. The simulation was run for 1.2 million years. The final sand geometry is shown in Fig. 4.

We found that, after 1.2 million years, a maximum hydrate saturation of 25% as achieved in the Orange sand at the base of the MHSZ (Fig. 5). Lower hydrate saturations are seen in the updip portion of the sand. These results suggest that diffusion alone may be able to form the observed hydrate deposits at WR313. However, we need to run additional simulations to analyze the effects of input parameters, mainly the rate of microbial methanogenesis.

Figure 4. Present-day geometry of the Orange sand used in simulation. Colors are contoured by depth. The dark blue surface is the base of the MHSZ.
Figure 5. Hydrate saturation in the Orange sand after 1.2 million years of sedimentation, microbial methanogenesis, and diffusive migration of methane into the sand. Color scale is hydrate saturation.

Task 4.2. To assess the role of advective methane supply in generating the observed features at WR313, we ran simulations in which methane-saturated water flows at a constant upward rate of 4 mm/yr through the domain, with no microbial methanogenesis. The domain and rock properties were the same as those used in the diffusion simulations. We found that the hydrate saturations achieved in these simulations were much lower than those achieved in the diffusion simulations. For example, after about 750,000 years, only about 1% hydrate saturation was observed in the sand, and the hydrate was not present throughout the sand the way it was in the diffusion simulations (Fig. 6). Much higher advection rates would be necessary to develop similar hydrate saturations. We are currently testing different parameters to assess the validity of our results.

Task 4.3. To assist with assessing the fluxes associated with different migration mechanisms and associated parameter space testing, we completed the development of a reaction-transport modeling method that accounts for porosity changes during compaction. The model uses numerical integration to compute steady-state dissolved methane concentrations and gas hydrate or gas bubble volume fractions as a function of depth in a one-dimensional geometry. The numerical method is computationally fast and is suitable for Monte Carlo simulations. In these simulations, model outputs are computed in a large number of iterations where uncertain input
parameters are allowed to vary within realistic limits. By retaining the results where the predicted gas hydrate amounts agree with observations, these Monte Carlo simulations measure the uncertainty in the input model parameters. The plan is to apply Monte Carlo simulation to quantify the uncertainty of the intensity and depth distribution of microbial methanogenesis. The results will be useful to constrain the contribution of microbial methanogenesis in the three-dimensional, time-dependent reservoir simulator that we have developed.

Specific objectives

None for this quarter.

Significant results and key outcomes

Our simulation results indicate that microbial methanogenesis and diffusive migration can yield significant hydrate saturations (25%) between the initial deposition of the Orange sand and the present day. In addition, advection needs to be much more rapid than we originally anticipated to allow similar accumulation without microbial methanogenesis.
What opportunities for training and professional development has the project provided?

PI Daigle and co-PI Mohanty have been working with PhD student Michael Nole and MS students Ryan Andris, Abhishek Bihani, and Arash Shushtarian on various aspects of pore-scale modeling of methane hydrate systems. This work has involved weekly meetings and independent work.

Co-PIs Cook and Malinverno have been working with PhD student Li Wei on modeling microbial methanogenesis. This work has involved weekly meetings and independent work.

How have the results been disseminated to communities of interest?

One peer-reviewed publication was submitted this quarter, and five abstracts were accepted for presentation at the American Geophysical Union Fall Meeting in December.

Plans during next reporting period to accomplish goals

Work will continue on Tasks 4.1, 4.2, and 4.3. In particular, we will focus on parameter space testing for diffusive and advective methane supply. This will involve permeability and pore size predictions from logs, and incorporating Monte Carlo simulations to constrain the most important input parameters.

PRODUCTS


PARTICIPANTS AND OTHER COLLABORATING ORGANIZATIONS

Name: Hugh Daigle
Project role: PI
Nearest person month worked: 1
Contribution to project: Project management; assisted with code development
Collaborated with individual in foreign country: No

Name: Kishore Mohanty
Project role: Co-PI
Nearest person month worked: 1
Contribution to project: Assisted with code development
Collaborated with individual in foreign country: No

Name: Steven Bryant
Project role: Co-PI
Nearest person month worked: 1
Contribution to project: Assisted with code development
Collaborated with individual in foreign country: No

Name: Michael Nole
Project role: Graduate Student
Nearest person month worked: 3
Contribution to project: Primary worker on developing computer code
Collaborated with individual in foreign country: No

Name: Abhishek Bihani
Project role: Graduate Student
Nearest person month worked: 1
Contribution to project: Capillarity and phase equilibrium modeling
Collaborated with individual in foreign country: No

Name: Arash Shushtarian
Project role: Graduate Student
Nearest person month worked: 1
Contribution to project: Sediment physical properties modeling
Collaborated with individual in foreign country: No

Name: Ryan Andris
Project role: Graduate Student
Nearest person month worked: 1
Contribution to project: Pore-scale diffusion modeling
Collaborated with individual in foreign country: No

Name: Ann Cook
Project role: Co-PI
Nearest person month worked: 1
Contribution to project: Worked on gathering specific data for modeling of microbial methanogenesis, developing methanogenesis code
Collaborated with individual in foreign country: No

Name: Li Wei
Project role: Graduate Student
Nearest person month worked: 3
Contribution to project: Worked on developing methanogenesis code
Collaborated with individual in foreign country: No

Name: Alberto Malinverno
Project role: Co-PI
Nearest person month worked: 1
Contribution to project: Provided data for microbial methanogenesis modeling
Collaborated with individual in foreign country: No
IMPACT

What is the impact on the development of the principal discipline of the project?

The central focus of this project is refining our understanding of the methane migration pathways that feed methane hydrate deposits in marine sediments. Understanding migration pathways is an important component of understanding methane hydrates as a petroleum system, a necessary step towards prospecting for economically recoverable hydrate deposits. Additionally, our results will help refine our understanding of the carbon cycle in marine sediments, and specifically how methane is transported and sequestered.

What is the impact on other disciplines?

The results of this project will be important for other engineering disciplines in which researchers are developing methods for extracting methane from the subsurface since it will provide information on how methane is distributed in sediments at different scales. In addition, the results will be of interest to the economics and risk assessment fields since we will develop methods to determine more precisely how much hydrate may be present in subsurface reservoirs.

What is the impact on the development of human resources?

This project will provide funding for three graduate students to conduct collaborative research on methane hydrates and give them an opportunity to participate in important hands-on learning experiences outside the classroom.

What is the impact on physical, institutional, and information resources that form infrastructure?

Our results may be used for better design of subsea oil and gas infrastructure since more precise assessment of hydrate resources will allow better assessment of hydrates as a hazard. In addition, production infrastructure specifically for hydrate reservoirs may be improved by our results since we will allow more accurate determination of the volumes of methane expected to exist in the subsurface.

What is the impact on technology transfer?

Our results will be disseminated at conferences and in peer-reviewed publications.

What is the impact on society beyond science and technology?
The impact of this work on society will be twofold. First, the better understanding of hydrates in a petroleum systems framework will allow for more efficient production of natural gas from these deposits, which will provide an additional energy resource. Second, the better understanding of methane cycling and distribution in the subsurface will influence regulatory decisions involving hydrates as geohazards or climate change agents.

**What dollar amount of the award’s budget is being spent in foreign country(ies)?**
None

**CHANGES/PROBLEMS**
None

**SPECIAL REPORTING REQUIREMENTS**
None

**BUDGETARY INFORMATION**
See attached spreadsheet.

Variances: Expenditures are within 80% of budget.

**References**


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