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
Prof. Hugh Daigle, PI
Phone: 512-471-3775
Fax: 512-471-9605
daigle@austin.utexas.edu

July 24, 2017

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 – March 31, 2018

REPORTING PERIOD END DATE: June 30, 2017

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 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 and hydrate 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
Completed 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
Completed 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
Completed 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

Daigle and graduate student Ryan Leung finished modeling capillary pressure effects at the base of the hydrate stability zone. In this zone, capillary effects cause hydrate, water, and gas to occupy distinct regions of the pore size distribution of the host sediment. Liu and Flemings (2011) presented the phase equilibrium model for this scenario (Figure 1). Because host sediments have a distribution of pore sizes, capillary effects cause the base of hydrate stability to be located at different depths in pores of different sizes. The result is a zone over which gas replaces hydrate as the phase occupying the largest pores.

In a gas-water system, the capillary pressure of the gas phase is related to the gas saturation by the capillary drainage curve. When hydrate, water, and gas are all present, the capillary pressure

![Figure 1.](image)

Left: solubility versus depth for different pore sizes near the base of the hydrate stability zone at Blake Ridge. Pore size range was constrained by mercury injection capillary pressure measurements. Middle: phase saturations over the three-phase zone. Right: conceptual model of phase distribution within the pore size distribution over the three-phase zone. At the top of the three-phase zone, hydrate occupies the larger pores and water occupies the smaller pores. As depth increases, the phase equilibrium conditions will allow gas to be stable in the largest pore (of size $r_{m}$). With increasing depth, gas replaces hydrate in the larger pores, until the base of the three-phase zone, at which the last hydrate disappears from the largest pore. The smallest pore occupied by hydrate above the three-phase zone has size $r_{h}^{L+H}$ while the smallest pore occupied by gas below the three-phase zone has size $r_{g}^{L+G}$. These pore sizes are not necessarily equal. Figures from Liu and Flemings (2011).
of the gas phase can be determined by considering the smallest pore size occupied by gas. Assuming that gas and hydrate compete equally for larger pores, and that gas and hydrate do not occupy the same pores, the smallest gas-filled pore corresponds to the minimum pore size occupied by gas at twice the gas saturation if only gas and water were present. This means that, at a given gas saturation in the three-phase zone, the gas capillary pressure will be larger than it would be at the same gas saturation in a two-phase case.

We applied this model to Blake Ridge and Hydrate Ridge as test cases since Liu and Flemings (2011) presented detailed phase equilibrium models of these locations combined with measured pore size distributions. In the future we will attempt to estimate pore size distributions at Walker Ridge to apply the model there.

We considered scenarios corresponding to 5 different methane abundances at each location: 8, 16, 24, 32, and 40 grams of CH$_4$ per dm$^3$ of pore volume. Gas saturations versus depth were taken from Liu and Flemings 2011. Figure 2 shows the saturations at each location for the cases of a three-phase zone as well as the case when the base of the hydrate stability zone is a discrete horizon.

**Figure 2.** Left: gas saturation versus depth at Blake Ridge. Right: gas saturation versus depth at Hydrate Ridge. In each plot, the straight lines correspond to the case of a discrete base of hydrate stability, while the curved lines correspond to the case of a three-phase zone. Blue: 8 g CH$_4$/dm$^3$ pore volume; cyan: 16 g CH$_4$/dm$^3$ pore volume; green: 24 g CH$_4$/dm$^3$ pore volume; yellow: 32 g CH$_4$/dm$^3$ pore volume; orange: 40 g CH$_4$/dm$^3$ pore volume.

In all cases, we calculated the capillary pressure of the gas phase and compared it to the minimum horizontal effective stress under hydrostatic conditions. If the gas-phase capillary pressure exceeds this value, then fracturing may occur (e.g., Daigle et al., 2011). We determined the horizontal effective stress following the method of Daigle et al. (2011) where the bulk density at each location (Ocean Drilling Program Sites 995 and 1250) was integrated and the hydrostatic pressure was subtracted. This yielded the vertical effective stress under hydrostatic
conditions; the horizontal effective stress under hydrostatic conditions was assumed to be 67% of this value (Daigle et al., 2011).

Figure 3 shows the results. In the case of Blake Ridge, the gas phase capillary pressure is enhanced in the three-phase case, but not even the greatest methane quantity yields a large enough gas saturation to risk fracturing. At Hydrate Ridge, in contrast, the capillary pressure is reduced in the three-phase case, and in the case of the lowest methane quantity (8 g CH₄/dm³ pore volume) this suppresses fracturing behavior. The two locations we studied therefore display opposite behavior. Blake Ridge is in very deep water (~2800 m) while hydrate ridge is much shallower (~800 m), and the pore size distribution at Blake Ridge is much broader than that at Hydrate Ridge, possible because of a greater abundance of bioclastic sedimentary content. Overall we expect Walker Ridge to behave more like Blake Ridge simply because of the water depth; however, the sediments at Walker Ridge will probably have relatively narrow pore size distributions. Future work will help test this further.

Figure 3. Comparison of gas-phase capillary pressure and minimum horizontal effective stress under hydrostatic conditions at Blake Ridge (left) and Hydrate Ridge (right). Curves are normalized to this latter value; a ratio of 1 is marked by a black, dashed line in each case, representing the fracturing criterion. Curves and colors are the same as in Figure 2.

Graduate student Michael Nole performed some simulations of hydrate growth rate throughout the hydrate stability zone at WR 313. Using sand units defined from seismic data, lithologic heterogeneities were populated through the hydrate stability zone, and a combination of microbial methanogenesis and compaction-driven flow was simulated. Methodology for the simulations is reported in Nole et al. (2017). Results are shown in Figure 4. Even when an external, deep source of methane is not present, hydrate at the base of the stability zone tends to accumulate preferentially in sands since this is where flow is focused. Hydrate in clay layers tends to form only in the shallow sedimentary column. The ramifications of these observations will be explored in future simulations that include multiphase flow.
Figure 4. Top: sand units identified from seismic data at WR313. Bottom: hydrate growth rates in response to microbial methanogenesis, lithologic heterogeneity, and compaction-driven flow entering the base of the hydrate stability zone. Microbial methanogenesis is the only methane source in this simulation. In the shallow sediments, microbial methanogenesis permits rapid hydrate growth in clay layers. Near the base of the hydrate stability zone, hydrate growth is largely restricted to sand layers where flow is focused, with a few interesting exceptions.
Malinverno continued work on developing a time-dependent reaction-transport model to predict gas hydrate contents and reviewed published studies of time-dependent organic carbon deposition in the northern Gulf of Mexico. The goal is to establish whether enhanced organic carbon deposition during glacial low-sea level periods can explain the occurrence of methane hydrates in discrete sediment intervals. We have changed the modeling approach slightly. Malinverno and Wei also worked together and selected a simple implicit finite difference method for the diffusion component after discovering unresolvable problems with the Crank Nicholson method surrounding the sand layer. We have kept the semi-lagrangian for the advection component.

Specific objectives

None for this quarter

Significant results and key outcomes

We found that, in shallow water settings, a three-phase zone at the base of hydrate stability can inhibit fracturing driven by gas pressure, while in deep water settings, a three-phase zone can promote fracturing behavior.

We found that, even when a deep source of methane is not present, focusing of compaction-driven flow in sands can drive recycled methane back into the hydrate stability zone.

What opportunities for training and professional development has the project provided?

PI Daigle worked with MS student Ryan Leung and PhD student Michael Nole 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?

Five presentations were made at the 9th International Conference on Gas Hydrates in Denver, CO at the end of June.

Plans during next reporting period to accomplish goals

Work will continue on Tasks 5.1, 5.2, and 5.3.
**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: Ryan Leung
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: Michael Nole
Project role: Graduate Student
Nearest person month worked: 1
Contribution to project: Primary worker on basin 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
Our progress slowed somewhat due to students Michael Nole and Li Wei taking partial leaves of absence this quarter.

SPECIAL REPORTING REQUIREMENTS
None

BUDGETARY INFORMATION
See attached spreadsheet.

References
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<td>$174,139</td>
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<td>$1,124,289</td>
<td>$294,237</td>
<td>$1,418,526</td>
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<td>$(96,574)</td>
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**Budget Period 2**

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<tr>
<th>Cumulative Total</th>
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<th>Q1</th>
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<th>Q4</th>
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<td>Q1</td>
<td>Q2</td>
<td>Q3</td>
<td>Q4</td>
<td>Q5</td>
<td>Q6</td>
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**Budget Period 3**

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