Oil & Natural Gas Technology

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Quarterly Research Performance Progress Report

(Period ending 03/31/2013)

Application of Crunch-Flow Routines to Constrain Present and Past Carbon Fluxes at Gas-Hydrate Bearing Sites

Project Period: October 1, 2012 – September 30, 2013

Submitted by:

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EXECUTIVE SUMMARY

In November 2012, Oregon State University initiated the project entitled: **Application of Crunch-Flow routines to constrain present and past carbon fluxes at gas-hydrate bearing sites.** This project aims to develop a modeling module that will include all important biogeo-chemical processes that need to be considered in a in a methane-rich environment. This module will be applied to data from several DOE-supported drilling expeditions (e.g., Cascadia margin in US, Ulleung Basin in south Korea, and K-G basin in India) to quantify the dynamics of me-thane at present day and in the past.

For the first quarter of the project (Jan to Mar), we aim to understand the biogeochemical cycling around the sulfate-methane-transition-zone (SMTZ) by a using a kinetic modeling ap-proach. The modeling module we developed is able to account for the changes in concentration and isotopic profiles of various dissolved and solid species. A preliminary version of this model was used to describe biogeochemical data collected from the K-G basin in India. More tests of the model in different regions (e.g. Ulleung Basin in East Sea) and assessment of the significance of some environmental factors are in progress and will be the primary focus for the rest of this quarter.

PROGRESS, RESULTS, AND DISCUSSION

A complete kinetic model was formulated during this quarter. The reactions considered in the model are listed in Table 1and illustrated in Figure 1. Our model considers not only carbon but also part of the sulfur cycle since these two elements are tightly connected around the SMTZ. We are currently working on simulating data from the K-H basin, and in the future will include data from the Ulleung Basin to assess the applicability of this model in different settings. Sensi-tivity tests to evaluate the significance of several environmental factors to the depth of SMTZ are also in progress. The following checklist summarizes our progress in this quarter:

Task	Subtasks	
TASK 1 SMTZ biogeo-chemical cy-cling	1.1 Adapt CrunchFlow code to accept (and simulate) carbon isotope data.	Done
	1.2 Set up the model framework: discretization of spatial and temporal modeling domain, species (primary, secondary, gas, and minerals) considered, and thermodynamic and kinetic database entries.	Done
	1.3 Verify and test model parameters with field observations.	Some tests in progress
	1.4 Compare the results from CrunchFlow with our previous box model and re-adjust the model if necessary.	Done
	1.5 Run sensitivity tests to evaluate significance of environ-mental variables in the of the resulting fraction of contribu-tions from each carbon cycling reactions, and effects on the SMTZ depth	In Pro-gress

CONCLUSION
The kinetic model that we proposed to develop to comprehensively describe the biogeochemical cycling around SMTZ is very close to its completion. The verification of the model with field data from different regions and sensitivity tests on several environmental factors are in progress and will be the focus for the rest of this quarter.

COST STATUS

MILESTONE STATUS

Title: Carbon cycling around the present SMTZ

Planned Date: Mar 1, 2013

Verification Method: Comparison with our previous box model and similar models published.

Status: This milestone is achieved during this quarter.

ACCOMPLISHMENTS
A CrunchFlow modeling routine is developed and ready to be applied in other regions for the purpose of understanding the biogeochemical cycling around the SMTZ. This model is the most comprehensive model to date and is expected to be highly applicable in other regions.

PROBLEMS OR DELAYS
None

PRODUCTS
→ This progress report
→ A kinetic model that is ready to apply in other region to describe the biogeochemical cycling around SMTZ.

Table 1

Homogeneous reactions	
Acid-base	$H_2O+CO_2 \rightarrow HCO_3^-+H^+$
	$HCO_3^- \rightarrow CO_3^{-2}+H^+$
	$NH_4^+ \rightarrow NH_{3(aq)}+H^+$
	$H_3PO_4 \rightarrow H_2PO_4^-$
	$H_2PO_4^- \rightarrow HPO_4^{-2}$
	$HPO_4^{-2} \rightarrow PO_4^{-3}$
	$H_2S_{(aq)} \rightarrow HS^-+H^+$
	$HS^- \rightarrow S^{-2}+H^+$
	$FeS_{(aq)} + H^+ \rightarrow HS^- + Fe^{+2}$
Gas-dissolvent	$CH_{4(g)} \rightarrow CH_{4(aq)}$
	$CO_{2(g)} \rightarrow CO_{2(aq)}$
	$H_2S_{(g)} \rightarrow H_2S_{(aq)}$
Aquatic redox	AOM: $CH_{4(aq)}+SO_4^{-2} \rightarrow HCO_3^-+HS^-+H_2O$
	CR: $HCO_3^- + H^+ + 4H_{2(aq)} \rightarrow CH_{4(aq)}+3H_2O$
Heterogeneous reactions	
Calcite	$Ca^{+2}+HCO_3^- \rightarrow CaCO_{3(s)}+H^+$
CH2O-SO4	$(CH_2O)_{106}(NH_3)_{16}(H_3PO_4) + 53SO_4^{-2} + 14H_2O + 14CO_{2(aq)} \rightarrow 53H_2S + 120HCO_3^- + 16NH_4^+ + HPO_4^{-2}$
CH2O-ME	$(CH_2O)_{106}(NH_3)_{16}(H_3PO_4) + 14H_2O \rightarrow 53CH_4 + 39CO_2 + 14HCO_3^- + 16NH_4^+ + HPO_4^{-2}$
Pyrite	$FeS_{(aq)} + 2H_2S_{(aq)} \rightarrow FeS_{2(s)} + 2H_{2(aq)}$

Figure 1

COST STATUS

The project was initiated 1 January 2013, as per stated in the proposal. No expenditures on this grant were incurred until then.   Salary for WeiLi Hong and Marta Torres have been paid during the January-March quarter in support of this effort.

MILESTONE STATUS

No milestone was reached during this quarter.

ACCOMPLISHMENTS

No accomplishment was made during the quarter.

PROBLEMS OR DELAYS PRODUCTS

None

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