Progress Report
July 1 – Sept 30, 2009
Agency: DOE NETL
Project title: Integrating Natural Gas Hydrates in the Global Carbon Cycle
Agency Award Number: DE-NT0006558

Executive Summary

During this quarter, we have addressed three aspects towards the improvement of our two-dimensional model for modeling the formation and stability of methane hydrates under the seafloor. (A) First, we have improved of the code so that it is more robust, more stable and more self-consistent. These improvements are allowing the modeling of higher sedimentation rates, higher organic carbon fractions, and a better understanding of the flow of dissolved methane and free gas as well as the carbonate-buffer chemistry at various depths under the seafloor. (B) Second, we have added capabilities to the code to model the sources of heat, due to the latent heats of methane hydrate and ice, as well as the heat generated by the consumption of organic carbon by methanogens. (C) Third, enhancements to the two-dimensional code have been made in order to compare the model output to predecessor one-dimensional models.

Approach

A) Several issues have been resolved which make the code more robust, more stable and more self-consistent.

First, we have resolved several issues which allow the code to run at higher sedimentation rates (i.e., 22 cm/kyr) and at higher levels of organic carbon in the sediments (i.e., 3.5% org C). We found and resolved an instability at high sedimentation rates due to the impinging river currents going to zero velocity at large ocean depths, which allowed the dumping of large amounts of fine-grained sediments at certain locations on the seafloor. We resolved this by imposing a lower limit on the ocean current velocity, due to random motions. We also found that the code for landslides on the seaslopes is not stable when we run the code at the highest spatial resolution (in the lateral direction), though the code works fine at half spatial resolution.

Second, we found and fixed two problems with the subroutines we added in the previous quarter for computing the detailed chemistry of dissolved carbon dioxide, alkalinity, pH, dissolved (bi)carbonate ions, and solid calcium carbonate. Both of these problems were found because the two-dimensional model with these new subroutines was predicting that the pH was reaching values as low as 4 near the bedrock, which is rather acidic and which implies that the carbonate buffer chemistry was failing.

The first problem was the extrapolative use of temperature-dependent dissociation constants for the carbonate buffer chemistry at sub-seafloor temperatures that were above 120 degrees Celsius (i.e., near the bedrock). The published values of dissociation constants are valid up to 40-50 degrees Celsius. We decided to use, for the time being, fixed values for these dissociation constants, so that these dissociation constants do not depend on temperature. We don’t expect that this approximation will change our results significantly. In the future, we can allow for the dissociation constants of the carbonate system to have their standard temperature dependence up to 40-50 degrees Celsius, with some yet-to-be-determined heuristic variation of these constants at higher temperatures.

The second problem was that there was too much dissolved calcium being produced near the bedrock. This was likely due to brief, localized numerical instabilities in the simulation layers next to the bedrock which led to extremely high values of the concentration of calcium dissolved in the porewaters. We solved this problem by putting an upper limit in the code at a very high value of the calcium concentration. This limit is much higher than the range of reasonable calcium values, so it is not an unnatural assumption to put into the model.

Third, when we impose periodic ice ages on our model, with the sea levels oscillating by 120 meters with a 100,000 year period, then those seafloor sediments which are periodically exposed to the cold atmosphere have unexpected profiles of methane emission. In these exposed sediments, methane tends to be released to the atmosphere at very high rates. This is due to a combination of factors, including the lowering of the solubility of methane in water when the hydrostatic pressure is low, the assumption of water-saturated sediments, and the absence of methanotrophy in unsaturated sediments in our model. Until we can further enhance our model to better account for these issues, we will focus on understanding the release of methane from the deeply-submerged ocean sediments.

(B) We have added capabilities to the code to handle the heat sources and sinks due to the latent heats of methane hydrate and ice as well as the heat generated when methanogens consume organic carbon. The code previously allowed only for the conductive diffusion of heat from the geothermal source at the bedrock through the sediments, and through the hydrate and ice deposits, and into the sea or atmosphere. Now, we can simulate the internal generation of heat as hydrate or ice freezes, as well as the internal absorption of (latent) heat as ice melts or hydrate dissociates. The improvement to the code involved the implicit numerical solution of the differential equation for heat transport with this extra heat source term. The model responds appropriately to these changes by requiring more time for ice or hydrate to change to/from the liquid phase. In recent simulations, this has reduced the simulated volume of the hydrate deposit at depth by ~20%. The heat generated by methanogens also appears to move the hydrate stability zone upwards in places by a few hundred meters, which is significant. We are currently investigating how robust these results are.

(C) In order to compare and validate the output of the two-dimensional model that we are developing to previous one-dimensional models (i.e., the model of Davies and Buffett), we have added hooks in our code so that it can run in a one-dimensional mode. These hooks include the disabling of both the two-dimensional sediment transport and the isostatic floating/rebound of the lithospheric sediments on the asthenosphere. In this model comparison, we found an error in our distinction of different types of porosity. When we fixed this error, the vertical profiles of porosity and permeability exhibited the expected clogging in the hydrate stability zone. In this comparison of our model with previous one-dimensional models, we still need to increase the vertical resolution of our model for the sake of a more detailed, quantitative comparison, but the first results are promising. The current 1D vertical profiles (of limited vertical resolution) of hydrate, free gas, temperature, permeability, etc., are well within the realm of possibility.

Future

The next steps for this project include:

1) Further validation of the code for the heat sources (latent heat and methanogenesis);
2) Further improvement in the vertical resolution of the 1D version of our model for model intercomparison purposes;
3) Investigating the impact of using a non-constant value for the organic carbon fraction of the sediments;
4) Adding the capability to simulate the emergence of high-permeability layers of sediment due to the erosion of large-grain sediments during low sealevels.