Progress Report
Agency: DOE NETL
Project title: Integrating Natural Gas Hydrates in the Global Carbon Cycle
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Report Period 4/1/10 to 6/30/10

Executive Summary

During this quarter, we have addressed a number of specific aspects towards the improvement of our two-dimensional model for modeling the formation and stability of methane hydrates under the seafloor. We have made significant changes to the advection schemes for the pore fluid, enabling the model to cope with high-permeability sediments without limiting the time step, and for the solid sediment, increasing the model resolution in the critical hydrate stability region and enabling the calculation of the total fluid velocity, relative to the sea floor and including the effects of pore water burial by the sediment advection. In addition, the geochemical treatment of the pore water carbonate system and a radioiodide tracer have been improved.

Approach

1. A limiter has been added to the advection scheme, restricting the flows based on the changes in pressure gradient that they would generate. Fields w_limited and u_limited show the extent of the flow limitation -- 1.0 means no limitation and 0.0 means complete limitation.

2. Based on the results of the flow limiter, two time stepping schemes have been developed and tested, a fast trial run scheme which uses the previous time step of 5 years, and a more accurate mode with time step of 0.25 years. The results were improved by turning off the bubble effect on pressure, Bubble_Pressure. In the trial mode, if the model time step is lengthened the porosity begins to show a kink at a change in grid spacing near the sediment surface (item #3).

3. An arbitrary number of initial stripes can be set, and these retain something like their initial thickness (actually, their solid_vol values) throughout the run. The current thickness of these stripes is about 200 meters; any thinner and the time step would have to be decreased. This improves model resolution near the sediment surface.

4. Two variables have been added to the output, w_darcy and w_tot. The first is self-explanatory, the second is relative to the sea floor. To do this (and item #3), the numerics of the solid advection was redone, so that the flows are consistently defined on the top faces of the cells, for example.

5. The CaCO3 / CaO system was redone, most particularly adding inneficient and kludgey code to put the CaCO3 system into equilibrium at all depths. Otherwise, I could get either CaCO3 or the anorthite/kaolinite system to relax toward their equilibria sensibly, but when both were turned on they either would not converge (omega_igneous asymptoting toward zero it looked like, at least long-term temporarily) or they would oscillate. This replaces the Ca limiter that the code had before.

6. A age tracer has been added to the solid sediment, because with item #3 the correspondence between stripe and age has been further relaxed.

7. Item #6 was used to add an age component to the respiration rate of biologically-labile POC. Interestingly, while most of the rate constants in the code have to be scaled to do a short-time trial run and get an idea of how the results will be for longer time, the organic carbon system adjusts itself to a faster duration run, because the sediment is younger and the carbon reacts faster, all by itself.

8. Item #6 was also used to fix the radio-iodine system, to get the isotopic ratio of the source from decaying POC. The iodine results are saved as an apparent iodine age in the netcdf output. The iodine age of pore water is older than the sediment age near the sediment surface, and younger than the sediment in the deepest porewater, because of diffusion I guess. The respiration rate is now much higher right near the sediment surface than it was before, because the sediment is younger there. It will be interesting to do comparitive runs with and without the age scaling, comparing the iodine results. Also to look at how the iodine age scales with sediment column age (run duration).

Future

The next steps for this project include:

1) Revising the transport of methane gas through the sediment, skipping for now the actual flow of the gas, in favor of a more parameterized approach that will not impact the numerical stability of the code or be itself affected by numerical instability.
2) The horizontal flow scheme has a flux-limiter, but it needs to be redesigned to enable anisotrophic permeability. Currently, if the horizontal permeability is higher than the vertical, the coupled horizontal-vertical flow system is prone to numerical instability. The scheme will involve a relaxation toward homogenizing the excess pressure along stripes, in regions of the grid where the permeability of the sediment is too high to resolve the Darcy flow within a time step computationally tractable time step of five years.