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Progress Report
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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 further general progress in making our code more robust, and exploring the effects of varying the various parameters in the model. In the next quarter, we plan to finalize and double-check the code, so that we can generate model runs that would form the basis for a journal publication.

The specific aspects towards the improvement of our model are as follows.

1) Addition of an Iodine-129 radioactive tracer;
2) Limiting of the speeds of methane gas bubbles and pore water;
3) Reduction of rate of the isostatic relaxation of the sediments;
4) Computation of non-dimensionalized profiles of the porosity and pore-water pressures in one (vertical) dimension;
5) The particulate organic carbon (POC) has been subdivided into 4 sub-component fractions for tracking purposes refractory, biogenic, S2, and S3.
6) The calcium-carbonate reaction and the igneous-weathering reaction now has a new 'flux limiting' restriction to only allow a fractional change to the dissolved calcium levels for each computational time step.
7) Determination of the pore-fluid velocities in the moving reference frames.
8) Addition of anisotropy to the permeability of the sediments.
9) Exploration of the options in our code for (a) demanding the horizontal flow of bubbles when the bubbles reach a 'vertical trap' (b) disabling or enabling the buoyancy of the methane gas bubbles.
10) Recently, a new option was added to the code to allow modeling what happens AFTER a 10-100 kyr epoch of 5°C global warming of the oceans.

Approach
In this quarter, we have worked on a number of aspects of the code:

1) We have added a tracer for radioactive iodine to the code, following Fehn & Snyder (2003), wherein we track I129 (half-life 15.7 Myrs) relative to total iodine. This radioactive iodine tracer can be used to infer age of the pore waters in the sediments.

2) We debugged code that allows for the limiting of the speeds of (a) methane gas bubbles and (b) pore water. This allows us to run the model with larger time steps (i.e. 5 years). It can be difficult to use larger time steps when we have more computational layers in the vertical direction.

For the nominal case of one new computational layer spawned at the bedrock every 5 Myrs, the limiting speed for the bubbles is currently set at 10 mm/yr, and the limiting speed for the pore water is 1 mm/yr. These maximum speeds are at least 10 times larger than the typical speeds of the components and about 10 times larger than the maximum sedimentation rate.

With this limiting of the fluid and bubble speeds, we can now simulate sediments that have porosities that reach above the 0.05 milliDarcy range. Previously, it was difficult to simulate sediments with such a high porosity.

We are still exploring the maximum fluid and gas speeds that would allow us to simulate the passive margin with a spawn period for the computational layer being in the range of 1.25-2.5 Myrs.

3) We debugged code for adding a time constant to the isostatic relaxation of the sediments relative to the 'floating line' defined by the density of the Earth's mantle. Now, instead of imposing instantaneous isostatic relaxation, which imposes the equilibrium state on the topographic profiles, we have a time constant of 10,000 computational time-steps, or 50 kyrs.

4) We debugged code and computed non-dimensionalized profiles of the porosity and pore-water pressures in one (vertical) dimension, in order to compare to prior analytical and computational work of Xin-She Yang 'Theoretical Basin Modeling' (2006) and others.

5) The particulate organic carbon (POC) has been subvided into 4 sub-component fractions for tracking purposes, as opposed to the previous 2 sub-component fractions (refractory and labile). This amounts to a subdivision of the labile fraction of the POC into three fractions: biogenic, S2, and S3. Each of these sub-fractions of the labile POC is allowed to be consumed at different rates by either biogenic (for biogenic POC) or abiogenic (for S2 POC or S3 POC) processes, with differing levels of methane being produced.

6) The code for the calcium-carbonate reaction and for the igneous-weathering reaction has been debugged. One major change here is the new 'flux limiting' restriction of these reaction rates to only allow a fractional change to the dissolved calcium levels for each computational time step. Previously, with nominal reaction rates, sometimes these reactions would over-consume the calcium in a given time step. Now, we limit the consumption or production of dissolved calcium to be less than 15% of the standing level of dissolved calcium in that grid element for each of the two reactions. This limit on the change in dissolved calcium effectively limits the changes the other chemical species involved the reactions as well.

7) Code was added and debugged for determining the pore-fluid velocities in the moving reference frames. The Darcy velocity of the pore fluids is computed from the pressure gradients. The vertical component of the Darcy velocity is always positive -- it is in the upwards direction. The vertical component of the Darcy velocity is then corrected for the fluid transfer rate between the computational layers. This new corrected velocity is most

often positive in the upper 1-2 km or so of the sediments, but tends to be negative in sediments that are closer to the bedrock. These are only tendencies, however. Depending on the sediment compaction rate, there can be regions of negative velocity near the sea floor. A second correction is also applied to the velocity, which involves subtracting off the motion of the grid cell relative to the sea floor. This correction of the pore-fluid velocities in the moving reference frames is important for assessing how much methane can escape from the sediment surface. If the velocities are negative, then it is impossible for dissolved methane to be transported upward.

8) We added and debugged anisotropy to the permeability of the sediments. This allows for greater flow rates of both pore fluids and gas bubbles in the horizontal direction. We have been able to run models with permeabilities that are 100 times greater in the horizontal direction than in the vertical direction. The aforementioned limitation on fluid and bubble speeds has been helpful in achieving this anisotropy level in our simulations. A mechanism for this is the preferential orientation of sediment grains horizontally.

9) We have explored further the option in our code for demanding the horizontal flow of bubbles when the bubbles reach a 'vertical trap'. This vertical trap is signaled by a reduction (instead of the normal increase) of the vertical bubble velocity as the bubbles move upwards. When this option for the horizontal flow of bubbles (when vertically trapped) is enabled, the escape rates of methane bubbles can increase considerably.

A similar exploration has shown that disabling the buoyancy of the methane gas bubbles can reduce significantly the transport rates of the methane as well as the vertical distribution of methane in the sediments.

10) Recently, a new option was added to the code to allow modeling what happens AFTER a 10-100 kyr epoch of 5°C global warming of the oceans. There are certain instabilities in the model during this 10-100kyr period of ocean warming. We added the option to look at what happens during long periods after the period of global warming, in order to assess how well the computational grid ‘heals’ after the instabilities were initiated. Maybe this can be used to assess how to better handle these instabilities in the code.

We can run the code further after the ‘WarmingFinish’ option with either a ‘CoolingAgain’ option or with a ‘NOT(CoolingAgain)’ option. The CoolingAgain option is to see how well the sediments heal after the warming period.

The NOT(CoolingAgain) option is to see how the system responds to an eternal Warming Period (lasting for 10-100Myrs). Does the system reach a steady state level of methane bubbles being released? Or does the escape rate of methane bubbles keep increasing? Or does the model break down?

Future

The next steps for this project include:

1) Finalizing and double-checking the code, so that we can generate model runs that would form the basis for a journal publication that we hope to submit soon.