Progress Report
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Executive Summary

We have improved the handling of dissolved tracers in the code, especially temperature which is now affected by the variable thermal diffusion as a function of sediment porosity and composition, and a tracer for chlorinity has been added. We have modified the code to allow changes in sea level, by permitting the sediment column to outcrop above sea level without crashing the code. We have written but not yet incorporated the calculations of $CaCO_3$ equilibrium state as a function of porewater alkalinity and DIC concentration, enabling us to track deposition of authigenic $CaCO_3$ or its dissolution as driven by sediment respiration or diagenesis reactions. We have written and tested calculations for de-watering of hydrated clays, releasing fluid in the subsurface.

Approach

Changes in sea level have a strong impact on the distribution and character of the sediment fan, and they are a primary process in the formation of permafrost deposits in the high latitudes, one of the key study areas for the project (the Arctic). When the sea level drops by tens of meters, some of the near-shore sediments are exposed to the air, affording different boundary conditions than the submerged sediments experience (for example, cold air temperatures in the Arctic). The processes that need to be added in order to do a full permafrost simulation are the effects of the latent of ice formation, and the effects of ice on the permeability of the sediment. We are currently working on these two tasks.

Authigenic $CaCO_3$ formation has an impact on methane dynamics as it tends to form where methane encounters sulfate (SO_4), the $CaCO_3$ cement eventually blocking further transport of methane. Authigenic $CaCO_3$ is also a distinctive tracer for the activity of the methane cycle, so the model predictions will eventually serve as a point of comparison with drill core data.

The de-watering of hydrated clays (i.e., montmorillonite → illite + fresh-water) has an impact on the fluid transport within the sediment column, which will impact the extent and abundance of methane hydrate in the subsurface; we regard it as a necessary process before the full-scale simulations can be done.

The thermal diffusivity is also crucial to get right. Water generally has a lower thermal diffusivity than do dry sediment grains. Just underneath the sea floor, the sediments are rather porous, with the pores filled with seawater. At depth, near the bedrock, the pore space is significantly reduced, meaning that there is less water to buffer the heat flow. An additive mixture model is used to compute the thermal diffusivity for mixture of dry sediment grains, water and hydrate. We have also coded to have other components in the mixture model, for example methane bubbles. The effect of the variable thermal diffusivity is that near the bedrock, the thermal diffusivity is lower, and near the sea floor, the thermal diffusivity is higher, by roughly a factor of two. At certain depths, where there is extra pore space (caused by the additional water from the clay dewatering), the thermal diffusivity increases by 20-40%. For the permafrost simulations, we are adding water ice as another component to the thermal diffusivity mixture model, which will have a significant effect on the flow of heat through the sediments.

Conclusions

We are continuing to build the basis model that will be used in the four archetype simulations in the research plan: the passive margin (our initial default simulation for model development), the Arctic (we're getting closer), an active margin (the initial model configuration has been done) and the Gulf of Mexico (which will require special insertion of salt domes, affecting the temperature, salinity, and flow structures in the pore fluid).