Response to RC1 Comments for

Placing constraints on submarine permafrost extent along the U.S. Beaufort Shelf using thermodynamic modeling

Ms. No: EGUSPHERE-2025-5529

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RC1: In this work, the set up of present day marine permafrost under the sea bed below a seafloor cable in the U.S. Beaufort Shelf is simulated using PFLOTRAN, by considering the mass and energy transfer within the seabed since the LGM, while taking into account of sea level variations. The performed simulations are challenging and the results are interesting, paving the way to the interpretation of the DATS data acquired offshore from Oliktok Point along the seafloor cable.

Meanwhile, the presentation of the modelling approach suffers of flaws and is sometimes not complete enough. Besides, I have a few technical concerns regarding the simulations themselves, especially the lack of convergence study. Figures should also be improved. **Thus I recommend a major revision of this manuscript.**

Author Response: We thank the reviewer for their thoughtful and constructive assessment of our manuscript. We appreciate the recognition that the simulations are challenging and that the results provide a useful framework for interpreting the DATS observations collected offshore of Oliktok Point. Our goal with this study was to establish physically based bounds on submarine permafrost extent along the U.S. Beaufort Shelf and to provide context for ongoing geophysical investigations.

We also appreciate the reviewer's detailed comments regarding the presentation of the modeling approach, the technical aspects of the simulations, and the quality of several figures. We agree that portions of the manuscript would benefit from additional clarification and expansion, particularly regarding the numerical implementation, model assumptions, and discussion of model sensitivity and limitations. In response, we have carefully considered each comment and will revise the manuscript accordingly to improve clarity, completeness, and overall presentation quality. Specific responses to each point are provided below.

Reviewer Comment: More details needed on the simulations set up – complete presentation of the simulation domains, of the boundary conditions, etc.

Author Response: We agree that additional detail regarding the simulation setup would improve clarity and reproducibility. In the revised manuscript, we will expand the description of the model domain, discretization, initialization procedure, and boundary conditions. We will also revise several figures to provide a clearer summary of the simulation configuration and boundary conditions.

Reviewer Comment: Minor problems of structures (e.g.: simulations described before simulator, Fig 2 commented after Fig 7)

Author Response: Based on your comments, we also think portions of the manuscript would benefit from improved organization and flow. In the revised manuscript, we will restructure several sections to address this, including the example you have provided.

Reviewer Comment: No convergence study provided. How do look the results when using twice finer discretizations (both in space and time)? By quantifying the discrepancies between the used simulations and the finer ones, one can estimate the truncation errors, and then make sure that these truncation errors do not create artifacts important enough to mislead the analysis of the results.

Author Response: We thank the reviewer for this important comment. While the HYDRATE mode in PFLOTRAN has previously been applied and validated in frozen sediment and permafrost-related simulations (Fukuyama et al., 2025), we agree that including some convergence analysis would strengthen the manuscript. In the revised manuscript, we will briefly summarize the results and validation outcomes of this previous study and perform simulations using finer discretization for a representative scenario to evaluate numerical sensitivity. These results will be incorporated either as a new figure in the main text or within the supplementary material.

Fukuyama, David Erik, Bigler, Lisa, Carty, Olin Rico, Jayne, Rick, Leone, Rosemary Claire, Smallwood, Chuck Randall, Stein, Joshua, Flemings, Peter, Garrett, Riley, Mills, Tanner, Farquharson, Louise, & Nicolsky, Dmitry (2025). Coupled Hydrological-Thermal-Biogeochemical Modeling for Predicting Arctic Carbon Emissions (CH4PACE). https://doi.org/10.2172/3028606

Reviewer Comment: 162: '2.1 model domain' The simulation set up (discretization, etc) should be described after the presentation of the simulation methods, because the first ones depend on the second ones.

Author Response: We agree with the reviewer that the organization of these sections can be improved. In the revised manuscript, we will restructure the Methods section so that the simulator and numerical approach are introduced prior to the detailed presentation of the model domain, discretization, and simulation setup.

Reviewer Comment: l 163-168: "Each geological model is discretized into ~560,000 grid cells on an irregular, Cartesian grid. Along the horizontal X-dimension, grid cell width is 20 m. In the vertical Z-dimension, the resolution varies, ranging from 1 m near the surface of the domain to 20 m at the bottom" The convergence study performed for establishing this grid should be briefly summarized here.

Author Response: We acknowledge a brief discussion of grid convergence is warranted in this section. In the revised manuscript, we will summarize prior convergence and validation work performed for this PFLOTRAN process mode (Fukuyama et al., 2025) and additionally include results from a simplified convergence analysis conducted for this study to demonstrate the sensitivity of the results to spatial and temporal discretization.

Reviewer Comment: l 183: Figure 4 shows three main classes of grid cell size. Why three? How do the depths of transition between these classes have been chosen?

Author Response: The variable vertical discretization was selected to balance computational efficiency with the need to adequately resolve the shallow subsurface, where the largest thermal gradients and ice saturation changes occur. The finest grid spacing was maintained near the seafloor to better resolve the temperature structure relevant to the DTS observations, while coarser discretization was applied at greater depths where little to no ice formation occurs throughout the simulations. We will clarify this rationale in the revised manuscript and additionally discuss the results of the discretization sensitivity analysis referenced above as it pertains to vertical discretization.

Reviewer Comment: l 196: How the values given in Table 1 have been chosen? Here the measurements or bibliographical used for grounding the choices of these values should be given. Besides, porosity of sand varies over 10% and porosity of clay varies over 60%, but in both cases permeability is kept constant, which looks contradictory. Why not using also depth-dependent permeability?

Author Response: We acknowledge that permeability likely evolves with depth and porosity in natural systems. However, for this first-order sensitivity study, representative bulk permeability values were prescribed for each lithology to isolate the primary thermodynamic controls on submarine permafrost extent while limiting additional poorly constrained parameters. In the revised manuscript, we will clarify this assumption and discuss its associated implications and limitations.

Reviewer Comment: L 207-211: Giving the initial conditions before the boundary conditions is confusing. For instance it makes difficult the understanding of the spin up. By the way, what means exactly a 'short' spin up?

Author Response: We agree with the reviewer that the ordering of these sections could be improved for clarity. In the revised manuscript, we will reorganize the discussion of the initial and boundary conditions to better describe the simulation workflow and initialization procedure. We additionally acknowledge that the phrase "short spin-up" is potentially misleading and will remove this wording. The intent was simply to describe the brief initial period during which the model transitions from uniform initial conditions (0.5 MPa and 1◦C) toward physically realistic pressure and temperature gradients imposed by the boundary conditions. This transient adjustment period is non-consequential to the final simulation results.

Reviewer Comment: L 216: First mention of Figure 2, after the comment of Figure 7. Figure 2 must be inserted here, or it must be commented earlier.

Author Response: Thanks for catching this error – we will address this in the revised manuscript.

Reviewer Comment: L 216-217: "These factors are applied at the top boundary of the model, establishing transient Dirichlet boundary conditions for pressure, temperature, and mass fraction of salt." Figure 2 does not give any information regarding mass fraction of salt.

Author Response: You are correct. We will remove that mention as it is inappropriate.

Reviewer Comment: L 227: Then why not also considering cases with the most probable value of geothermal heat flux, 66 mW.m^{-2}?

Author Response: The selected geothermal heat flux values were intended to bound the reported regional average of 66 ± 14 mW m^{-2} rather than reproduce a single preferred condition. The averaged contours presented throughout the manuscript were included to provide an approximate representation of intermediate conditions near the reported mean geothermal heat flux.

Reviewer Comment: L 229-230: "For the lateral boundaries of the model domain, hydrostatic pressure and Dirichlet boundary conditions for the mass fraction of salt are applied." The presentation of the simulation domains and boundary conditions is weak. For instance, what is the value for the lateral Dirichlet boundary conditions for the mass fraction of salt? A figure summarizing the geometry and the full set of boundary conditions for all primary variables (temperature, pressure and mass fraction of salt) should be provided.

Author Response: As previously acknowledged, we agree that a more representative figure summarizing the model geometry, boundary conditions, and primary variables is needed to improve clarity. In the revised manuscript, we will expand the description of the imposed boundary conditions, and add a schematic figure summarizing the thermal, pressure, and salinity boundary conditions throughout the model domain.

Reviewer Comment: L 243: I guess D_α should also be indexed with respect to the component index j. If all the components are assumed to have the same diffusion coefficient, it should be specified and the errors associated to this simplifying assumption should be briefly discussed.

Author Response: In the revised manuscript, we will clarify the notation associated with the diffusion coefficient term and explicitly state that the same diffusion coefficient was assumed for all components in these simulations. We will additionally acknowledge this as a simplifying assumption and briefly discuss its associated limitations.

Reviewer Comment: L 244: wrong writing, '$q_\alpha$for α = l, g' would be better.

Author Response: Noted – we will address in the revised manuscript.

Reviewer Comment: L 246: What formulation is used for the relative permeabilities k_α^r – Brooks-Corey, van Genuchten, anything else? This information should be given here.

Author Response: The simulations utilized Mualem–van Genuchten relative permeability functions for both the liquid and gas phases within PFLOTRAN HYDRATE mode. In the revised manuscript, we will explicitly describe these constitutive relationships and provide the associated parameterization used in the simulations.

Reviewer Comment: L 249: Considering equation (4),

1) what S_α stand for? Only s_α is introduced in the text.
2) It seems that heat conduction is considered to happen only in the solid phase ('the rock'). Of course conduction occurs in all the phase of the porous medium, solid, ice, liquid, hydrate and gas. Is this a typo or a simplifying assumption? In the latter case the associated errors should be briefly discussed.
3) the heat capacity C_p looks also only computed by taking into account the solid phase. Same remark that for heat conduction.

Author Response: Good catch on 1, and thanks for the questions on 2 & 3. We agree that the notation and description of Equation (4) require clarification. In the revised manuscript, we will correct the inconsistency between sα and Sα and define all variables consistently.

We will also revise the description of heat conduction and heat capacity. The current wording oversimplifies the PFLOTRAN implementation by referring only to "rock" properties. In the simulations, material-specific dry and wet thermal conductivities are assigned for each lithology and used to represent effective thermal behavior of the porous medium. We will clarify this implementation and distinguish between the rock heat capacity and the effective multiphase thermal properties used in the energy balance.

Reviewer Comment: L 253-256 : "The phase transition between fully liquid-saturated and partially gas-saturated is handled by a conditional that checks the dissolved gas mole fraction; if its value exceeds solubility, a gas phase forms, and the primary variables switch to gas pressure, gas saturation, and temperature." Then I understand that in partially saturated conditions, an assumption is made regarding the flow of the liquid phase, so that the two-phase flow may still be described by a single-equation model. What is this assumption? It should be reminded here.

Author Response: We thank the reviewer for this comment. We agree that the description of the phase-switching behavior in PFLOTRAN HYDRATE mode should be clarified. In the revised manuscript, we will expand this section to more clearly describe the assumptions and numerical treatment associated with the transition between single-phase and two-phase conditions.

Reviewer Comment: L 259-260 : "and **a** parameter defined in Grenier et al. 2018." Please say explicitly which parameter. "and **the parameter X** defined in …"

Author Response: Okay, we will fix this in the revised manuscript. Thanks.

Reviewer Comment: Figure 11: The permafrost profiles inferred from the geophysical observations should be included in this Figure. The lithological logs should also be reminded alongside each simulations, to ease the interpretation of vertical variations.

Author Response: We thank the reviewer for this suggestion. We agree that including the interpreted geophysical permafrost profiles and lithologic logs alongside the simulations could aid interpretation of

Figure 11, and we will explore incorporating these additions in the revised manuscript. However, if these additions substantially reduce figure readability or introduce excessive visual complexity, we may retain the current layout and instead clarify these comparisons more explicitly within the text.

Reviewer Comment: Figure 12: it seems that there is a problem of legend – no red dashed lines, but grey ones instead. More importantly, I think that here observed resistivity should be presented as well, for allowing visual comparison between observations and simulation results.

Author Response: Oh, great catch on the legend issue. We will fix that. Same as for figure 11, we will consider the incorporation of the observed resistivity in this figure as that is a good idea, but if it impacts readability we may choose to exclude. Although, in this case it seems less of a concern as it would just be one additional line.

Reviewer Comment: L 400-404 : "Our research suggests that this signal … which may be misinterpreted as additional permafrost." Here the formulation should be clarified. At the beginning the presence of hydrocarbons seems hypothetical ('attributable'), while at the end it seems demonstrated ('indicates'). It can't be both at the same time.

Author Response: We thank the reviewer for identifying this inconsistency in wording. We agree that the discussion should more clearly distinguish between demonstrated model results and interpretation-based hypotheses. In the revised manuscript, we will revise this section to consistently frame deep hydrocarbon presence as a possible explanation for the observed high-resistivity signals rather than as a demonstrated conclusion.

Reviewer Comment: L 406-409 : "By comparing these temperature profiles with real DTS data, assessments regarding the accuracy of the DTS measurements and determinations of whether they fall within a realistic temperature range can be made." Indeed, comparison between observed and simulated temperature would be of great interest.

Author Response: We look forward to presenting these results in a separate manuscript. We are happy to hear it will be of great interest!

Reviewer Comment: L 413 : typo '?'

Author Response: Yes, thanks for catching this. Both the "?" and "–" should be removed and "a" should be capitalized as this is the start of a new sentence.

Reviewer Comment: L 416 : 'Frederick et al, 2026 (in prep)' – references to not already published work should be avoided.

Author Response: We thank the reviewer for this comment and agree that references to unpublished work should be minimized. In the revised manuscript, we will remove or revise this citation and instead refer more generally to the companion work within the PEMDATS scope.

Reviewer Comment: L 419-420: "The greatest variation is observed within the first 5 km of each model (Figure 13), where the shallow water depth makes the bottom water more sensitive to seasonal air temperature changes." I don't understand – these are modelling results, right? At line 220, it is specified that "When sections of the transect become submerged [...] a temperature of -1 ◦ C is applied." Then how could seasonal variations come into play?

Author Response: Another good catch and we thank the reviewer for identifying this unclear wording. The simulations do not incorporate seasonal temperature variability, as a constant submerged boundary temperature of −1◦C is prescribed. The intended point was that shallow-water regions are more strongly influenced by transitions between exposed and submerged conditions throughout the glacial-interglacial cycle, rather than by seasonal variability. We will revise this text to clarify the source of the modeled temperature variations.