

RESEARCH ARTICLE

Modeling freezing and BioGeoChemical processes in Antarctic sea ice

Raghav Pathak¹  | Seyed Morteza Seyedpour^{1,2} | Bernd Kutschen³ |
Andrea Thom¹ | Silke Thoms³ | Tim Ricken^{1,2} 

¹Institute of Structural Analysis and Dynamics in Aerospace Engineering, Faculty of Aerospace Engineering and Geodesy, University of Stuttgart, Stuttgart, Germany

²Porous Media Lab, Institute of Structural Mechanics and Dynamics in Aerospace Engineering, Faculty of Aerospace Engineering and Geodesy, University of Stuttgart, Stuttgart, Germany

³Ecological Chemistry, Alfred Wegener Institute, Bremerhaven, Germany

Correspondence

Raghav Pathak, Institute of Structural Analysis and Dynamics in Aerospace Engineering, Faculty of Aerospace Engineering and Geodesy, University of Stuttgart, Stuttgart 70569, Germany.
Email:
raghav.pathak@isd.uni-stuttgart.de

Funding information

Deutsche Forschungsgemeinschaft, Grant/Award Numbers: 463296570, 312860381, 390740016, 436883643, 327154368, 504766766, 465194077; Federal Ministry of Education and Research, Grant/Award Number: 031L0304A

Abstract

The Antarctic sea ice, which undergoes annual freezing and melting, plays a significant role in the global climate cycle. Since satellite observations in the Antarctic region began, 2023 saw a historically unprecedented decrease in the extent of sea ice. Further ocean warming and future environmental conditions in the Southern Ocean will influence the extent and amount of ice in the Marginal Ice Zones (MIZ), the BioGeoChemical (BGC) cycles, and their interconnected relationships. The so-called pancake floes are a composition of a porous sea ice matrix with interstitial brine, nutrients, and biological communities inside the pores. The ice formation and salinity are both dependent on the ambient temperature. To realistically model these multiphasic and multicomponent coupled processes, the extended Theory of Porous Media (eTPM) is used to develop Partial Differential Equations (PDEs) based high-fidelity models capable of simulating the different seasonal variations in the region. All critical variables like salinity, ice volume fraction, and temperature, among others, are considered and have their equations of state. The phase transition phenomenon is approached through a micro-macro linking scheme. In this paper, a phase-field solidification model [4] coupled with salinity is used to model the microscale freezing processes and up-scaled to the macroscale eTPM model. The evolution equations for the phase field model are derived following Landau-Ginzburg order parameter gradient dynamics and mass conservation of salt allowing to model the salt trapped inside the pores. A BGC flux model for sea ice is set up to simulate the algal species present in the sea ice matrix. Ordinary differential equations (ODE) are employed to represent the diverse environmental factors involved in the growth and loss of distinct BGC components. Processes like photosynthesis are dependent on temperature and salinity, which are derived through an ODE-PDE coupling with the eTPM model. Academic simulations and results are presented as validation for the mathematical model. These high-fidelity models eventually lead to their incorporation into large-scale global climate models.

This is an open access article under the terms of the [Creative Commons Attribution](https://creativecommons.org/licenses/by/4.0/) License, which permits use, distribution and reproduction in any medium, provided the original work is properly cited.

© 2024 The Author(s). *Proceedings in Applied Mathematics & Mechanics* published by Wiley-VCH GmbH.

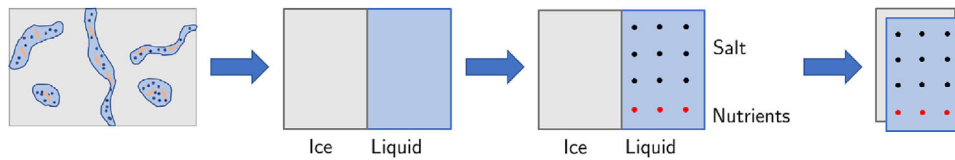


FIGURE 1 Homogenization of the mixture body.

1 | INTRODUCTION

Recent severe fluctuations in the Southern ocean sea ice extent call for an urgent need of better understanding of the seasonal physical and BioGeoChemical (BGC) processes occurring within the sea ice. Sea ice is affected by several environmental factors like temperature, wind patterns, and ocean salinity, among others.

The sea ice microstructure is highly complex, composed of a solid ice matrix with fluid interstitial brine inclusions. Microbial communities find the brine inclusions nutrient rich habitats for their growth and survival during the harsh winter months. The growth, or photosynthetic rate of microbial communities is dependent on various environmental factors like temperature, sunlight, brine salinity, and nutrient availability. While satellite observations and large scale modeling has brought better understanding of these processes on large scales (>1 km), there still lies a gap in the exact temporal description of small scale processes like ice freezing and its coupling to biogeochemistry.

In this paper, a mathematical framework in the extended Theory of Porous Media (eTPM) to model thermodynamically consistent freezing process is developed on the macroscale (≈ 1 m). The formation of pores and dendritic patterns is resolved on a 1D microscale (≈ 0.1 mm) model and the pore area is upscaled to the macroscale to regulate ice growth rate. The algal growth is model using a N-P single nutrient and phytoplankton (N-P) growth model. The current work follows further from ref. [1], improved by microscale mass exchange between ice volume fraction and brine, description of evolution of bulk salinity through partial differential equation, and coupled ordinary differential equations for primary production and nutrient dynamics.

2 | THEORETICAL FRAMEWORK

In this section all important physical and BGC process occurring within the sea ice are modeled. Firstly, processes related to ice physics, like volume fraction of ice and brine, brine salinity, temperature, and pore properties are presented in the Subsection 2.1. In the next Subsection 2.2, a single N-P model is presented with different considerations for environmental conditions.

2.1 | Sea ice physics

The eTPM [2–4] presents a method for modeling heterogeneous materials using the concept of volume fractions, where miscible components φ^β can exist within the immiscible macro phases φ^α . The overall homogenized mixture body φ can then be written as

$$\varphi = \bigcup_{\alpha}^{\kappa} \varphi^{\alpha} := \bigcup_{\alpha}^{\kappa} \left(\bigcup_{\beta}^{\nu} \varphi^{\alpha\beta} \right), \quad (1)$$

where $\alpha = 1, \dots, \kappa$ are the number of immiscible phases, denoted by φ^α and $\beta = 1, \dots, \nu$ are the miscible phases, denoted by $\varphi^{\alpha\beta}$. For sea ice, the immiscible phases of solid ice matrix and liquid brine are denoted as $\alpha = \mathbf{I}, \mathbf{L}$ and the liquid phase further consists of dissolved salts and water, given as $\varphi^{\mathbf{L}\beta}$ with $\{\beta = \mathbf{s}, \mathbf{w}\}$. Through an averaging procedure the true structure is homogenized into a smeared continua as shown in Figure 1. The amount of each constituent present in the control domain is described using the concept of volume fraction given as

$$n^{\alpha} = \frac{dv^{\alpha}}{dv}, \quad (2)$$

where n^α is the volume fraction, given as ratio of partial volume of the phase dv^α with respect to the volume of the total volume dv .

For modeling purposes, the sea ice is assumed to be an isothermal biphasic material with an incompressible solid ice matrix. The density changes in ice and brine can; however, occur due to temperature and brine salinity, respectively. Considering the saturation condition for interactions between phases, the following relations are determined.

$$\theta = \theta^\alpha, \quad \rho^{\text{IR}} = \rho^{\text{IR}}(\theta), \quad \rho^{\text{LR}} = \rho^{\text{LR}}(S^{\text{br}}), \quad \sum_{\alpha} \hat{\rho}^\alpha = 0, \quad \sum_{\alpha} \hat{\mathbf{p}}^\alpha = \mathbf{0}, \quad \sum_{\alpha} \hat{\mathbf{e}}^\alpha = \mathbf{0}, \quad (3)$$

where S^{br} is the salinity of brine trapped within the pores in ice, and $\hat{\rho}^\alpha, \hat{\mathbf{p}}^\alpha, \hat{\mathbf{e}}^\alpha$ are the mass, momentum and energy interactions between the phases α . Applying necessary and evaluating the Clausium–Duhem entropy inequality yields the restrictions on constitutive relations. The weak forms of the balance equations can be written by integrating over the control domain B_I w.r.t solid phase. The mathematical operators of divergence and gradient are defined as $\text{div}(\bullet) = \nabla \cdot (\bullet) = \frac{\partial(\bullet)}{\partial x_i} \cdot \mathbf{e}_i$ and $\text{grad}(\bullet) = \nabla \otimes (\bullet) = \frac{\partial(\bullet)}{\partial x_i} \otimes \mathbf{e}_i = \nabla(\bullet) = \frac{\partial(\bullet)}{\partial x_i} \mathbf{e}_i$, and the rate of change of a given quantity w.r.t time is given by $(\bullet)'_I$. The balance equations can then be written as

- Mass balance of ice

$$\int_{B_I} \left\{ (n^{\text{I}})'_I \rho^{\text{IR}} + n^{\text{I}} (\rho^{\text{IR}})'_I \text{tr} \mathbf{D}_I - \hat{\rho}^{\text{I}} \right\} \delta n^{\text{I}} dv = 0, \quad (4)$$

where use has been made of the relation $\text{tr} \mathbf{D}_I = \mathbf{D}_I \cdot \mathbf{I} = \text{grad} \mathbf{x}'_I \cdot \mathbf{I} = \text{div} \mathbf{x}'_I$.

- Concentration balance of salt

$$\begin{aligned} & \int_{B_I} \left\{ n^{\text{L}} (S^{\text{br}})'_I + (n^{\text{L}})'_I S^{\text{br}} + \frac{n^{\text{L}}}{\rho^{\text{LR}}} S^{\text{br}} (\rho^{\text{LR}})'_I + n^{\text{L}} S^{\text{br}} \text{tr} \mathbf{D}_I \right\} \delta S^{\text{bulk}} dv \\ & - \int_{B_I} \left\{ \frac{\mathbf{j}^{\text{LS}}}{\rho^{\text{LR}}} \cdot \text{grad} \delta S^{\text{bulk}} \right\} dv = \int_{\partial B_I} \left\{ \frac{\mathbf{j}^{\text{LS}}}{\rho^{\text{LR}}} \delta S^{\text{bulk}} \cdot \mathbf{n} \right\} da, \end{aligned} \quad (5)$$

where \mathbf{j}^{LS} is the total salt flux as a result of advective and diffusive components, given as $\mathbf{j}^{\text{LS}} = \mathbf{j}^{\text{LS}}_{\text{adv}} + \mathbf{j}^{\text{LS}}_{\text{dif}}$.

- Mass balance of mixture

$$\begin{aligned} & \int_{B_I} -\{n^{\text{L}} \mathbf{w}_{\text{LI}} \cdot \text{grad} \delta p^{\text{LR}}\} dv + \int_{B_I} \left\{ \text{tr} \mathbf{D}_I + \sum_{\alpha} \frac{n^{\alpha}}{\rho^{\alpha R}} (\rho^{\alpha R})'_I \right. \\ & \left. - \hat{\rho}^{\text{I}} \left(\frac{1}{\rho^{\text{LR}}} - \frac{1}{\rho^{\text{IR}}} \right) \right\} \delta p^{\text{LR}} dv = - \int_{\partial B_I} \{n^{\text{L}} \mathbf{w}_{\text{LI}} \delta p^{\text{LR}} \cdot \mathbf{n}\} da, \end{aligned} \quad (6)$$

where \mathbf{w}_{LI} is the Darcy velocity of the pore fluid.

- Momentum balance of mixture

$$\int_{B_I} \left(\sum_{\alpha}^{\text{IL}} \mathbf{T}^\alpha \right) \cdot \text{grad} \delta \mathbf{u}_I dv - \int_{B_I} \left(\sum_{\alpha}^{\text{IL}} \rho^\alpha \right) \mathbf{b} \cdot \delta \mathbf{u}_I dv = \int_{\partial B_I} \{ \mathbf{t} \cdot \delta \mathbf{u}_I \} da, \quad (7)$$

where \mathbf{T}^α is the partial Cauchy's stress tensor and \mathbf{b} is the body force.

- Energy balance of mixture

$$\begin{aligned} & \int_{B_I} \left\{ \theta \rho^{\text{I}} (\eta^{\text{I}})'_I \right\} \delta \theta dv + \int_{B_I} \left\{ \theta \rho^{\text{L}} (\eta^{\text{L}})'_L \right\} \delta \theta dv - \int_{B_I} \{ \mathbf{q} \cdot \text{grad} \delta \theta \} dv \\ & + \int_{B_I} \{ \hat{\mathbf{p}}^{\text{I}} \cdot \mathbf{w}_{\text{LI}} \} \delta \theta dv + \int_{B_I} \{ \hat{\rho}^{\text{I}} [\mathbf{h}^{\text{L}} - \mathbf{h}^{\text{I}}] \} \delta \theta dv = \int_{\partial B_I} \{ \mathbf{q} \delta \theta \cdot \mathbf{n} \} da, \end{aligned} \quad (8)$$

where η^I and η^L are the partial specific entropies of ice and liquid phases, and $(h^L - h^I)$ is the latent heat of phase change due to freezing. A coupled phase field model [5] is used to describe the phase transition between ice and liquid on the microscale. The evolution of microscale ice volume fraction and salinity are given as

$$\begin{aligned} \tau \frac{\partial n_{\text{Micro}}^I}{\partial \tau} &= -\frac{\delta \varphi_{LG}}{\delta n_{\text{Micro}}^I} = -\frac{\partial \varphi_L}{\partial n_{\text{Micro}}^I} + \varepsilon^2 \frac{\partial^2 n_{\text{Micro}}^I}{\partial \zeta^2} \\ &= -n_{\text{Micro}}^I + \frac{3}{2} n_{\text{Micro}}^I{}^2 - \left(\frac{1}{2} - \left(m - \frac{1}{2} \sigma \right) \right) n_{\text{Micro}}^I + \varepsilon^2 \frac{\partial^2 n_{\text{Micro}}^I}{\partial \zeta^2} \\ \tau \frac{\partial \sigma}{\partial \tau} &= -\frac{\partial^2}{\partial \zeta^2} \left(\frac{\delta \varphi_{LG}}{\delta \sigma} \right) = \varepsilon^2 \frac{\partial^2}{\partial \zeta^2} \left(\frac{1}{4} n_{\text{Micro}}^I{}^2 + \beta \sigma \right), \end{aligned} \quad (9)$$

where n_{Micro}^I , and σ are the dimensionless microscale ice volume fraction and bulk salinity, respectively. ε , and β are the constants determining the length of transition region between ice and salt, and m is a temperature dependent constant determining the freezing point depression and is given as $m = \frac{1}{2} \frac{T - T_s}{T_0 - T_s}$. The macroscale growth rate is determined following [6] given as

$$\rho^I = a_{\Gamma} \frac{(\mathbf{q}^L - \mathbf{q}^I) \cdot \mathbf{n}_{\Gamma}}{(h^L - h^I)}, \quad (10)$$

where a_{Γ} is the pore area, \mathbf{q}^L and \mathbf{q}^I are the heat fluxes of ice and liquid, and \mathbf{n}_{Γ} is the normal direction vector of gradient of temperature.

2.2 | Sea ice BioGeoChemistry

The N-P BGC model assumes a single algal species and a single nutrient [7]. The equation for carbon concentration due to algae is given as

$$\left(C_C^{\text{Alg}} \right)'_{\text{I}} = \left(\hat{\rho}_{\text{Alg}}^{\text{gpp}} - \hat{\lambda}_{\text{Alg}}^{\text{loss}} \right) C_C^{\text{Alg}}, \quad (11)$$

where $\hat{\rho}_{\text{Alg}}^{\text{gpp}}$ and $\hat{\lambda}_{\text{Alg}}^{\text{loss}}$ denote the growth and loss term of algae, respectively. The growth is dependent on the Photosynthetically Active Radiation (PAR), Nutrient availability, brine salinity, and temperature. The growth rate is determined following [8, 9] and is given as

$$\hat{\rho}_{\text{Alg}}^{\text{gpp}} = \hat{\rho}_{\text{Alg,max}}^{\text{gpp}} F_{\text{PAR}} F_{\text{N}} F_{\text{S}} F_{\theta}, \quad (12)$$

where F_{PAR} , F_{N} , F_{S} , F_{θ} are the regulating functions of their respective environmental factors. The loss rate of algae is given as a constant fraction of growth rate

$$\hat{\lambda}_{\text{Alg}}^{\text{loss}} = 0.1 \times \hat{\rho}_{\text{Alg}}^{\text{gpp}}. \quad (13)$$

Finally, the rate of change of Nutrient is given as

$$\left(C_C^{\text{N}} \right)'_{\text{I}} = r_C^{\text{N}} \left(-\hat{\rho}_{\text{Alg}}^{\text{gpp}} + f_{\text{rm}} \hat{\lambda}_{\text{Alg}}^{\text{loss}} \right) C_C^{\text{Alg}}, \quad (14)$$

where r_C^{N} and f_{rm} are the stoichiometric ratio and a factor to accommodate remineralization from ocean, respectively. In the present case both are set to 1 since there is only one nutrient and no interactions with ocean are considered.

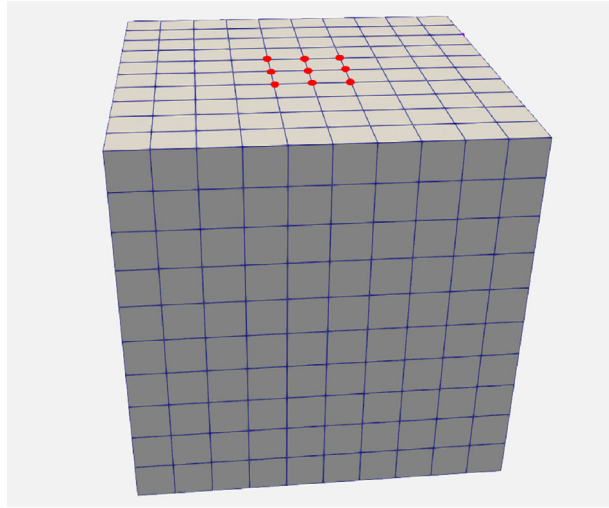


FIGURE 2 IBVP. IBVP, initial boundary value problem.

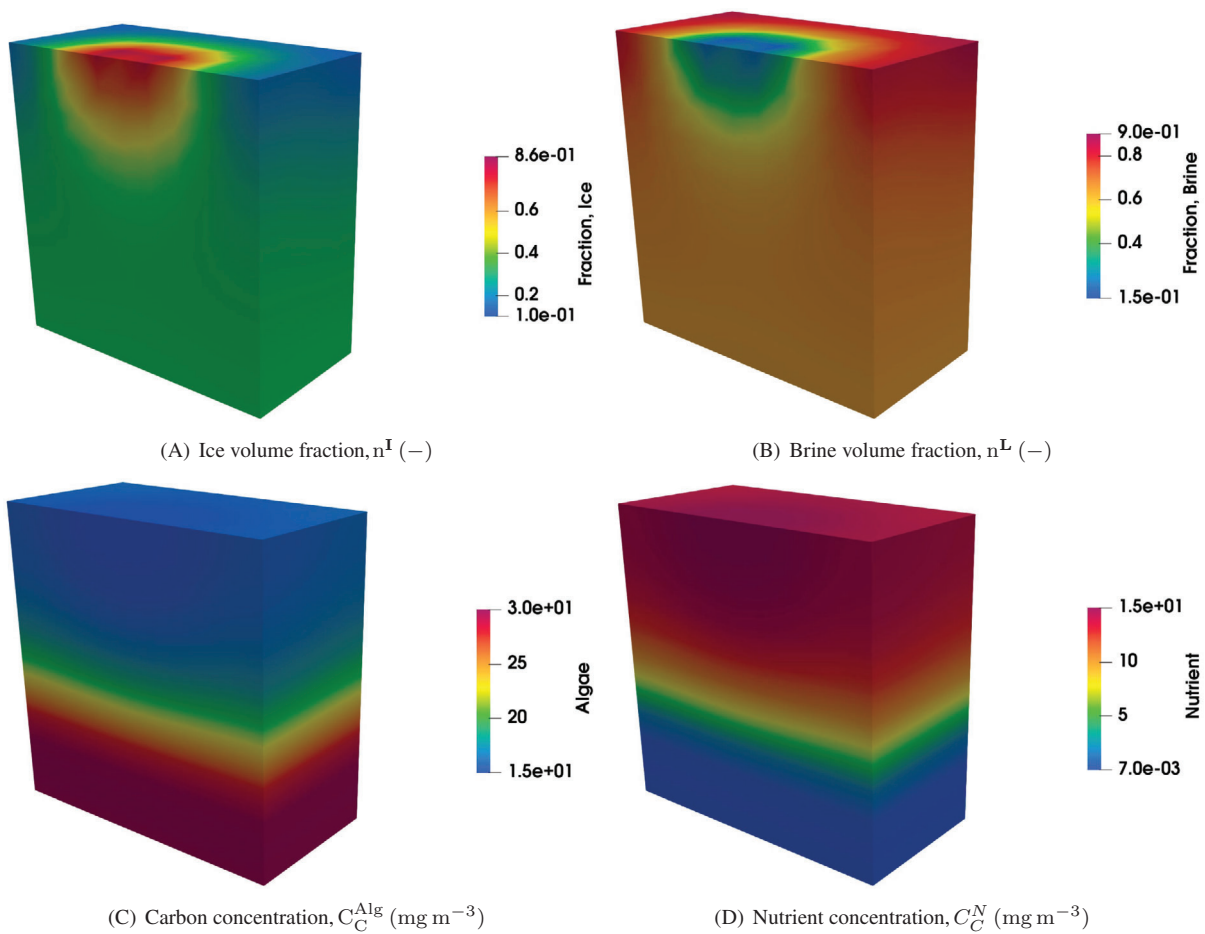


FIGURE 3 Temporal evolution of physical and BGC variables. BGC, biogeochemical.

3 | RESULTS

The Initial Boundary Value Problem (IBVP) is set considering physical conditions in the Antarctic MIZ. A low temperature of -12°C is prescribed on nine nodes at the top surface considering the cold atmospheric temperatures as shown in Figure 2. The rest of the domain has an initial temperature of -1.8°C which is in reasonable agreement with typical

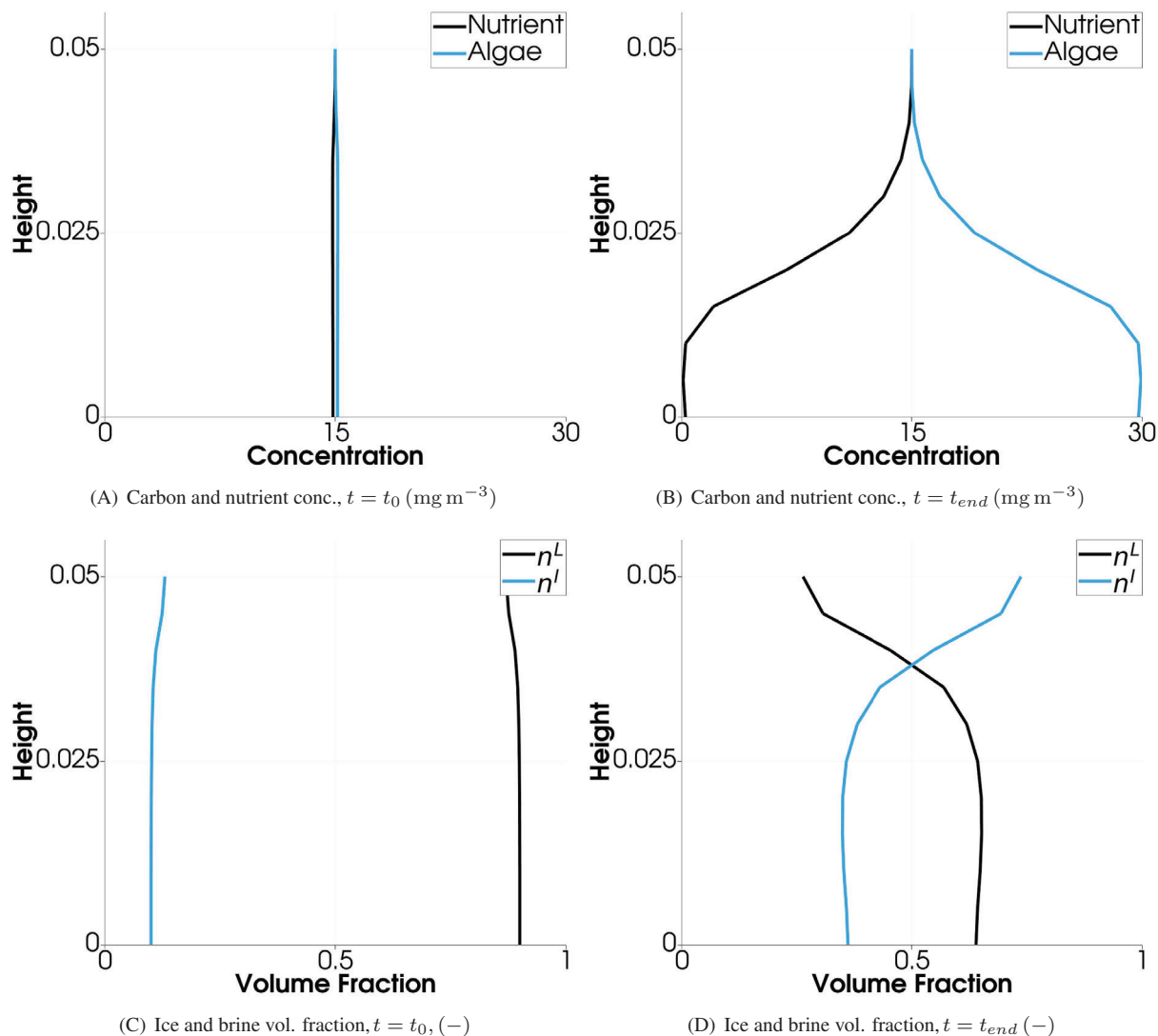


FIGURE 4 Evolution along height.

seawater temperatures. Bulk salinity is prescribed to be 35 *ppt* in the entire domain and brine salinity is calculated based on the temperature using the relation $S^{\text{br}} = -21.4\theta - 0.886\theta^2 - 0.0170\theta^3$. The time evolution of key quantities is observed at the central cut section of the cubical domain and is presented in Figure 3.

It can be clearly observed that with time the volume fraction of ice is higher on the top of the control domain and the algal concentration is higher at the bottom. This can be attributed to low atmospheric temperatures at the atmosphere-ocean interface which leads to ice growth from the top. As the ocean water has warmer temperature than the upper ice layers, algae starts forming at the bottom of ice. The available nutrients are used up by the algae and hence a height dependent plot in Figure 4 shows the simultaneous growth and loss of carbon and nutrient between the initial and final times. The ice and brine volume fractions are also presented.

4 | CONCLUSIONS

This paper presents a multiscale, multiphase, and multicomponent coupled physical and BGC model to simulate sea ice growth and carbon production due to algal species living within the brine channels in the ice. On the macroscale eTPM is employed to model the multiphase and multicomponent nature of sea ice incorporating ice, brine, and salt dynamics. The size of pores and growth of ice is motivated from the microscale coupled phase field solidification model. The primary

production and BioGeoChemistry is modeled using various environmental factors like temperature, salinity, light, and nutrients. Academic simulations are presented to prove the utility of the developed modeling framework. The developed high fidelity model brings a possibility to be incorporated into large scale global climate models.

ACKNOWLEDGMENTS

This work was supported by the Deutsche Forschungsgemeinschaft (DFG) in the framework of the priority program SPP 1158 “Antarctic Research with comparative investigations in Arctic ice areas” by the following grant 463296570 (Priority Programme SPP 1158, Antarctica). T.R. further thanks the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) for supporting this work via the following projects: 312860381 (Priority Program SPP 1886, Subproject 12); 390740016 (Germany’s Excellence Strategy EXC 2075/1); 436883643 (Research Unit Programme FOR 5151 (QuaLiPerF), Project P7); 327154368 (SFB 1313 Project C03 Vertebroplasty); 504766766 (Project Hybrid MOR); 465194077 (Priority Programme SPP 2311, Project SimLivA). TR is further supported by the Federal Ministry of Education and Research (BMBF, Germany) within ATLAS by grant number 031L0304A.

Open access funding enabled and organized by Projekt DEAL.

ORCID

Raghav Pathak  <https://orcid.org/0009-0008-6495-5814>

Tim Ricken  <https://orcid.org/0000-0001-8515-5009>

REFERENCES

1. Thom, A., & Ricken, T. (2021). In silico modeling of coupled physical-biogeochemical (P-BGC) processes in Antarctic sea ice. In: *Proceedings in Applied Mathematics and Mechanics*, 20. <https://doi.org/10.1002/pamm.202000308>
2. Ricken, T., Sindern, A., Bluhm, J., Widmann, R., Denecke, M., Gehrke, T., & Schmidt, T. C. (2014). Concentration driven phase transitions in multiphase porous media with application to methane oxidation in landfill cover layers. *Zeitschrift für Angewandte Mathematik und Mechanik*, 94, 609–622.
3. Seyedpour, S. M., Thom, A., & Ricken, T. (2023). Simulation of contaminant transport through the vadose zone: A continuum mechanical approach within the framework of the extended theory of porous media (eTPM). *Water*, 15(2), 343. <https://doi.org/10.3390/w15020343>
4. Seyedpour, S. M., Henning, C., Kirmizakis, P., Herbrandt, S., Ickstadt, K., Doherty, R., & Ricken, T. (2023). Uncertainty with varying subsurface permeabilities reduced using coupled random field and extended theory of porous media contaminant transport models. *Water*, 15(1), 159. <https://doi.org/10.3390/w15010159>
5. Thoms, S., Kutschan, B., & Morawetz, K. (2013). Phase-field theory of brine entrapment in sea ice: Short-time frozen microstructures. *arXiv: Atmospheric and Oceanic Physics*. <https://doi.org/10.48550/arXiv.1405.0304>
6. Ehlers, W., & Häberle, K. (2016). Interfacial mass transfer during gas–liquid phase change in deformable porous media with heat transfer. *Transport in Porous Media*, 114, 525–556. <https://doi.org/10.1007/s11242-016-0674-2>
7. Vancoppenolle, M., & Tedesco, L. (2017). *Numerical models of sea ice biogeochemistry*. Wiley. <https://doi.org/10.1002/9781118778371.ch20>
8. Tedesco, L., Vichi, M., & Thomas, D. N. (2012). Process studies on the ecological coupling between sea ice algae and phytoplankton. *Ecological Modelling*, 226, 120–138.
9. Geider, R. J., MacIntyre, H., & Kana, T. M. (1998). A dynamic regulatory model of phytoplankton acclimation to light, nutrients, and temperature. *Limnology and Oceanography*, 43, 679–694.

How to cite this article: Pathak, R., Seyedpour, S. M., Kutschan, B., Thom, A., Thoms, S., & Ricken, T. (2024). Modeling freezing and BioGeoChemical processes in Antarctic sea ice. *Proceedings in Applied Mathematics and Mechanics*, e202400047. <https://doi.org/10.1002/pamm.202400047>