

MODELING SMALL SCALE PROCESSES IN ANTARCTIC SEA ICE

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Summary. The Antarctic sea ice, which undergoes annual freezing and melting, plays a significant role in the global climate cycle. Adverse environmental conditions in the Southern Ocean influence the extent and amount of ice in the Marginal Ice Zones (MIZ), the BioGeo- Chemical (BGC) cycles, and their interconnected relationships. The 'Pancake' floes are a composition of porous sea ice matrix with interstitial brine, nutrients, and biological communities inside the pores. To realistically model these multi-phasic and multi-component coupled processes, the extended Theory of Porous Media (eTPM) is used to develop models capable of simulating the different seasonal variations. 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. A Phase-field solidification model coupled with salinity is used to model the micro-scale freezing processes and up-scaled to the macro scale eTPM model. This allows for modeling the salt trapped inside the pores. For the biological part, a BGC flux model for sea ice is also set up to simulate the algal species present in the sea ice matrix. Processes like photosynthesis are dependent on temperature and salinity, and 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 will eventually lead to their incorporation into large-scale global climate models.

1 INTRODUCTION

Sea ice plays an important role in the global climate. The recent drastic variations in the extent of sea ice in the Southern Ocean necessitate an immediate and improved understanding of the seasonal physical and biogeochemical processes within the sea ice. Environmental variables such as temperature, wind patterns, and ocean salinity influence the highly heterogeneous and complex microstructure of sea ice, comprising a solid ice matrix interspersed with fluid brine inclusions. These brine inclusions serve as nutrient-rich habitats for microbial communities,

facilitating their growth and survival during the severe winter months. The growth or photosynthetic rate of these microbial communities is also severely influenced by various environmental factors such as temperature, sunlight, brine salinity, and nutrient availability.

While satellite observations and large-scale modeling have enhanced our understanding of these processes on larger scales (greater than 1km), there still remains a gap in the precise temporal description of small-scale processes like ice freezing and its linkage to biogeochemistry.

This paper presents a mathematical framework within the extended Theory of Porous Media (eTPM) to model a thermodynamically consistent freezing process on the macroscale (approximately 1m). The formation of pores and dendritic patterns is resolved on a 1D microscale (approximately 0.1mm) model, and the pore area is upscaled to the macroscale to regulate the ice growth rate. The thermodynamic growth of sea ice also affects the mechanical properties of ice, such as Young's and bulk moduli and the Poisson's ratio. The algal growth is modeled using ordinary differential equations considering key processes like photosynthesis, lysis, exudation and respiration.

2 THEORETICAL FRAMEWORK

This section starts with establishing the model equations for the physical and biogeochemical dynamics of growing winter first year sea ice. In subsection 2.1, the equations for evolution of various critical variables like ice and brine volume fractions, salinity, deformations, and temperature are set up using the mass balance of ice, mass balance of mixture, momentum balance of mixture, and the energy balance of mixture. Equations for evolution of mechanical properties of first year granular sea ice are also discussed. In subsection 2.2, the equation for growth of ice algae are described along with critical environmental variables.

2.1 Sea ice physics using extended Theory of Porous Media (eTPM)

The fundamentals of the Theory of Porous Media (TPM) are derived from the integration of two primary concepts: the theory of mixtures and the concept of volume fractions. These foundational principles enable a detailed consideration of the local composition within the overall aggregate. The Extended Theory of Porous Media (eTPM) [1, 2, 3, 4] offers a comprehensive approach for dealing with miscible substances φ^β that are present within immiscible macroscopic phases φ^α . The aggregate φ is composed of κ macroscopic phases, denoted as φ^α , with $\alpha = 1, \dots, \kappa$. Furthermore, each immiscible phase can consist of ν components $\varphi^{\alpha\beta}$, which are identified and transported within phase φ^α . The overall aggregate mixture body can then be homogenized as $\varphi = \bigcup_{\alpha}^{\kappa} \varphi^\alpha := \bigcup_{\alpha}^{\kappa} \left(\bigcup_{\beta}^{\nu} \varphi^{\alpha\beta} \right)$. For the description of sea ice as a biphasic aggregate the ice and seawater are resolved as immiscible phases, $\varphi^{\mathbf{I}}$ and $\varphi^{\mathbf{L}}$ respectively with the seawater phase being a mixture of salt and water, given as $\varphi^{\mathbf{L}\beta}$ with $\{\beta = s, w\}$, designated as salt (s) and freshwater (w), respectively.

The physical and mechanical properties of sea ice vary with changing sea ice microstructure due to freezing. The temperature driven Young's and Shear moduli and Poisson's ratio are given as

$$\begin{aligned} E(\theta) &= 8.93 + 1.2e - 2(\theta_m - \theta)\text{GPa} \\ G(\theta) &= 3.41 + 4.5e - 3(\theta_m - \theta)\text{GPa} \\ \mu(\theta) &= 0.308 + 7e - 5(\theta_m - \theta), \end{aligned} \tag{1}$$

where θ_m and θ are the melting temperature of ice and ambient temperature, respectively. The balance equations for the description of porous sea ice can be written as

- Mass balance of ice

$$\int_{\mathbf{B}_I} \left\{ (\mathbf{n}^I)'_{\mathbf{I}} \rho^{\mathbf{IR}} + \mathbf{n}^I (\rho^{\mathbf{IR}})'_{\mathbf{I}} \text{tr} \mathbf{I} - \hat{\rho}^{\mathbf{I}} \right\} \delta \mathbf{n}^{\mathbf{I}} \text{d}v = 0, \quad (2)$$

- Concentration balance of salt

$$\begin{aligned} & \int_{\mathbf{B}_I} \left\{ \mathbf{n}^{\mathbf{L}} (\mathbf{S}^{\text{br}})'_{\mathbf{I}} + (\mathbf{n}^{\mathbf{L}})'_{\mathbf{I}} \mathbf{S}^{\text{br}} + \frac{\mathbf{n}^{\mathbf{L}}}{\rho^{\mathbf{LR}}} \mathbf{S}^{\text{br}} (\rho^{\mathbf{LR}})'_{\mathbf{I}} + \mathbf{n}^{\mathbf{L}} \mathbf{S}^{\text{br}} \text{tr} \mathbf{D}_I \right\} \delta \mathbf{S}_{\text{Macro}}^{\text{bulk}} \text{d}v \\ & - \int_{\mathbf{B}_I} \left\{ \frac{\mathbf{j}^{\text{Ls}}}{\rho^{\mathbf{LR}}} \cdot \text{grad} \delta \mathbf{S}_{\text{Macro}}^{\text{bulk}} \right\} \text{d}v = \int_{\partial \mathbf{B}_I} \left\{ \frac{\mathbf{j}^{\text{Ls}}}{\rho^{\mathbf{LR}}} \delta \mathbf{S}_{\text{Macro}}^{\text{bulk}} \cdot \mathbf{n} \right\} \text{d}a, \end{aligned} \quad (3)$$

- Mass balance of mixture

$$\begin{aligned} & \int_{\mathbf{B}_I} - \left\{ \mathbf{n}^{\mathbf{L}} \mathbf{w}_{\text{LI}} \cdot \text{grad} \delta \mathbf{p}^{\mathbf{LR}} \right\} \text{d}v + \int_{\mathbf{B}_I} \left\{ \text{tr} \mathbf{D}_I + \sum_{\alpha} \frac{\mathbf{n}^{\alpha}}{\rho^{\alpha \mathbf{R}}} (\rho^{\alpha \mathbf{R}})'_{\mathbf{I}} \right. \\ & \left. - \hat{\rho}^{\mathbf{I}} \left(\frac{1}{\rho^{\mathbf{LR}}} - \frac{1}{\rho^{\mathbf{IR}}} \right) \right\} \delta \mathbf{p}^{\mathbf{LR}} \text{d}v = - \int_{\partial \mathbf{B}_I} \left\{ \mathbf{n}^{\mathbf{L}} \mathbf{w}_{\text{LI}} \delta \mathbf{p}^{\mathbf{LR}} \cdot \mathbf{n} \right\} \text{d}a, \end{aligned} \quad (4)$$

- Momentum balance of mixture

$$\int_{\mathbf{B}_I} \left(\sum_{\alpha} \mathbf{T}^{\alpha} \right) \cdot \text{grad} \delta \mathbf{u}_I \text{d}v - \int_{\mathbf{B}_I} \left(\sum_{\alpha} \rho^{\alpha} \right) \mathbf{b} \cdot \delta \mathbf{u}_I \text{d}v = \int_{\partial \mathbf{B}_I} \left\{ \mathbf{t} \cdot \delta \mathbf{u}_I \right\} \text{d}a, \quad (5)$$

- Energy balance of mixture

$$\begin{aligned} & \int_{\mathbf{B}_I} \left\{ \theta \rho^{\mathbf{I}} (\eta^{\mathbf{I}})'_{\mathbf{I}} \right\} \delta \theta \text{d}v + \int_{\mathbf{B}_I} \left\{ \theta \rho^{\mathbf{L}} (\eta^{\mathbf{L}})'_{\mathbf{L}} \right\} \delta \theta \text{d}v - \int_{\mathbf{B}_I} \left\{ \mathbf{q} \cdot \text{grad} \delta \theta \right\} \text{d}v \\ & + \int_{\mathbf{B}_I} \left\{ \hat{\mathbf{p}}_{\text{E}}^{\mathbf{I}} \cdot \mathbf{w}_{\text{LI}} \right\} \delta \theta \text{d}v + \int_{\mathbf{B}_I} \left\{ \hat{\rho}^{\mathbf{I}} [\mathbf{h}^{\mathbf{L}} - \mathbf{h}^{\mathbf{I}}] \right\} \delta \theta \text{d}v = \int_{\partial \mathbf{B}_I} \left\{ \mathbf{q} \delta \theta \cdot \mathbf{n} \right\} \text{d}a. \end{aligned} \quad (6)$$

Microscale freezing is modeled using coupled volume fraction and bulk salinity on the microscale and upscaled on the macroscale following [5]. The macroscale growth term is taken following an interfacial mass exchange process [6] as

$$\hat{\rho}^{\mathbf{I}} = a_{\Gamma}(\mathbf{n}_{\text{Micro}}^{\mathbf{I}}) \frac{(\mathbf{q}^{\mathbf{L}} - \mathbf{q}^{\mathbf{I}}) \cdot \mathbf{n}_{\Gamma}}{(\mathbf{h}^{\mathbf{L}} - \mathbf{h}^{\mathbf{I}})}, \quad (7)$$

where $a_{\Gamma}(\mathbf{n}_{\text{Micro}}^{\mathbf{I}})$ is upscaled from the microscale as pore area dependent on the microscale volume fraction.

2.2 Primary production in sea ice

Ice algae living within the brine pores during winters act as primary producers, converting inorganic carbon dioxide to organic carbon and making it available for other organisms living in the ice and ocean environments. The Gross Primary Production (GPP) in sea ice is modeled following [7], where the production rate is dependent on ambient environmental conditions of temperature, salinity, sunlight and nutrient availability. The total production is given as

$$\hat{\rho}_{Alg}^{gpp} = \hat{\rho}_{Alg,max}^{gpp} F_{\theta} F_s F_{PAR} F_N, \quad (8)$$

where F_{θ} , F_s , F_{PAR} , and F_N are limiting functions for temperature, salinity, light and nutrient, respectively. These functions lie between 0 and 1 and regulate the GPP variations by acting as prefactors to the maximum possible growth. The limiting functions are given as

$$\begin{aligned} F_{\theta} &= (Q_{10}^{Alg})^{\frac{\theta-10}{10}}, \\ F_s &= \exp \left[- \left(2.16 - 8.3 \times 10^{-5} \cdot (S^{br})^{2.11} - 0.55 \ln(S^{br}) \right)^2 \right], \\ F_{PAR} &= 1 - e^{-\frac{E_{PAR}}{E_k}}, \\ F_n &= \frac{I^n}{I^n + d_n}. \end{aligned} \quad (9)$$

Finally, carbon assimilation is given as

$$\left(C_C^{Alg} \right)' = \hat{\rho}_{Alg}^{gpp} \cdot C_C^{Alg}. \quad (10)$$

3 Results

The results are evaluated on a cuboidal domain with the upper boundary acting as an interface between atmosphere and ocean and a prescribed Dirichlet temperature BC is given on the nodes considering realistic conditions in the sea ice zone. The rest of the domain is prescribed with an initial condition of seawater temperature of 272 K. The bottom layer is prescribed with a dirchlet BC on Bulk salinity as 35 ppt representing the average salinity of seawater. For the biogeochemical dynamics, the initial carbon concentration is set to 10 mg. The simulation is run for 24 hours, considering a full day. The IBVP can be seen in fig. 1.

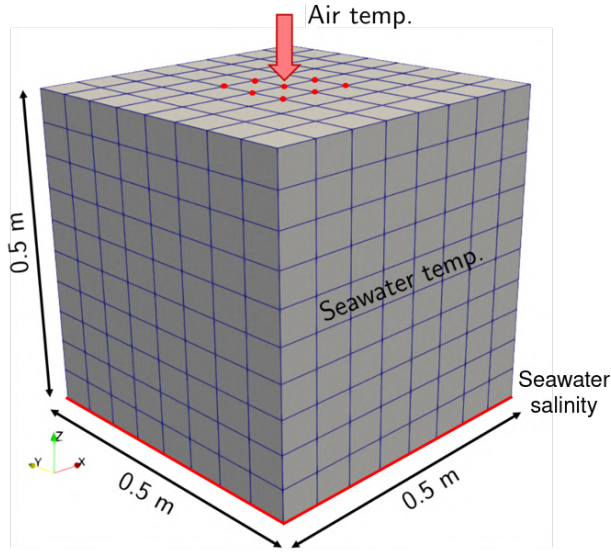


Figure 1: Boundary value problem for simulation

3.1 Sea ice physics

Thermodynamical freezing of the seawater column is presented in fig. 2. Owing to the constraint applied by saturation condition, it is observed that as the seawater freezes, the ice volume fraction in the domain increases, and hence, resulting in a decrease in liquid volume fraction. Temperature distribution is along the depth also shows lower values on the upper layers, that are usually exposed to the atmosphere, and as the depth increases, temperature increases as well and the ice volume fraction decreases.

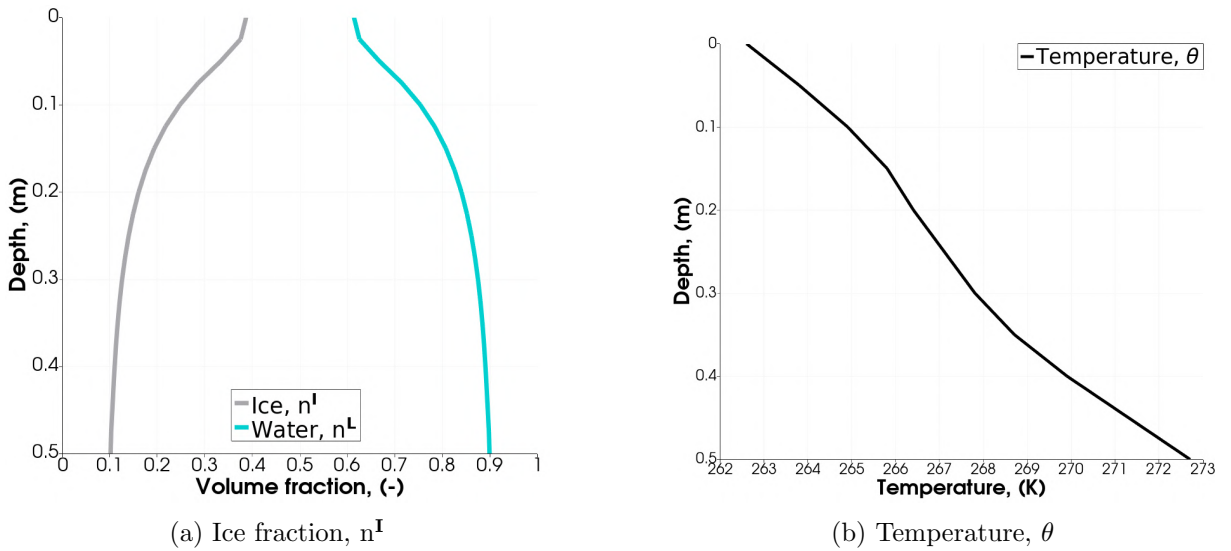


Figure 2: Ice and temperature dynamics during a 24 h freezing simulation

With growing sea ice, the physical and mechanical properties also change. The Young's and bulk moduli, and Poisson's ratio of ice increases due to consolidation of crystals. Fig. 3 shows the increase in mechanical constants of sea ice due to freezing of seawater, indicating an increase in strength of the ice column.

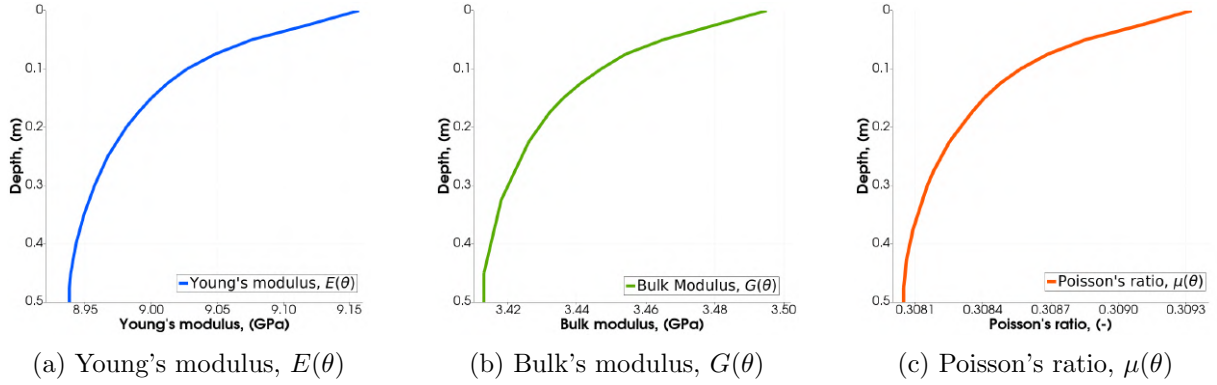


Figure 3: Change in physical properties of ice during a 24 h freezing simulation

3.2 Sea ice BioGeoChemistry

The carbon concentration change is presented in fig. 4. It is observed that due to adverse environmental conditions on the upper regions of the domain, a lower concentration is reported and increases further down as the depth increases due to better temperature, and salinity conditions.

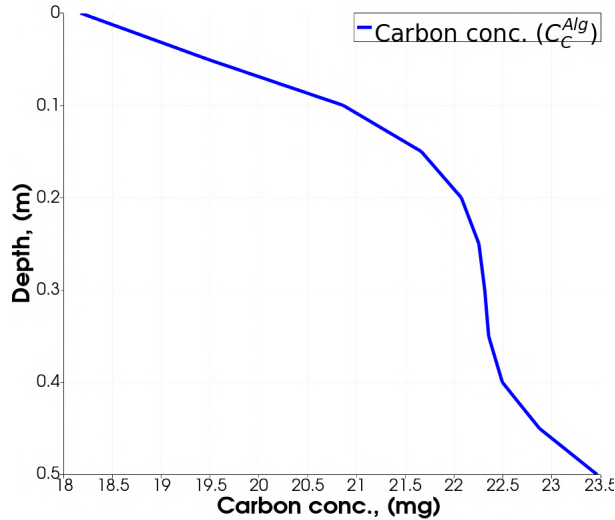


Figure 4: Accumulated carbon by ice algae during a 24 h freezing simulation

Parameters space for light, and temperature are rather well defined from observational data, and well established salinity- temperature relations in sea ice govern the salinity dependence. There are, however, multiple nutrients that affect the photosynthesis, and their availability also depends on several factors like seasonal variations, geographical locations, ocean currents

and extent of sea ice cover, among others. It becomes important to analyse the dependence on nutrients availability on carbon concentration. Three critical macronutrients, namely, Silica, Nitrogen, Phosphorous are analysed following (9)(d). The half saturation constants for the three nutrients are given as $d_N = 1.6 \mu\text{M}$, $d_{Si} = 3.9 \mu\text{M}$, and $d_P = 0.24 \mu\text{M}$ [8]. The ranges for nutrient availability for all three nutrients are taken as $0.01 \mu\text{mol}$, $0.1 \mu\text{mol}$, $1 \mu\text{mol}$, $10 \mu\text{mol}$, $100 \mu\text{mol}$. The results show that, while the extreme ends of the parameter ranges do not show large differences, the nutrient values in the middle tend to severely affect the carbon concentration. This is due to the fact that the values are very close to the limits of 0 and 1. For $0.01 \mu\text{mol}$, $F_N = 0.006$, $F_{Si} = 0.002$, and $F_P = 0.02$ and for $100 \mu\text{mol}$, the limiting values are calculated as $F_N = 0.984$, $F_{Si} = 0.962$, and $F_P = 0.997$. The extremal values, however, are still important as they might influence unusual behaviors, such as in fig. 5b, where growth is observed on the upper layers of the domain even though other environmental factors like temperature, and salinity are adverse.

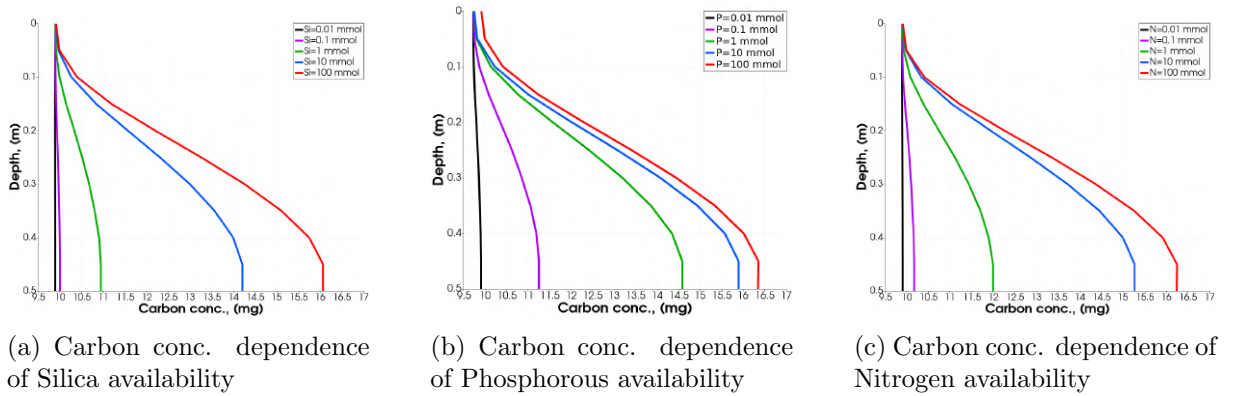


Figure 5: Nutrient limitation on carbon concentration during a 24 h freezing simulation

4 CONCLUSIONS

In this paper, a modeling framework is presented using the extended Theory of Porous Media (eTPM) for the macroscale, phase field model for microscale phase separation and rate depending quota based photosynthesis model for primary production and carbon assimilation in sea ice. The change in physical properties of sea ice and biological activity during a 24 h simulation run with freezing is discussed in detail. The effect of nutrient availability on carbon assimilation by ice algae is modeled and analysed. However, at present it is difficult to conclude if one nutrient is more critical than others for overall primary production. In the future, models with various stoichiometric ratios of Silica, Nitrogen and Phosphorous could be analysed. Nutrient limitation term itself could also be parametrized to incorporate more than one nutrient at a given simulation instance.

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