

A FRAMEWORK FOR MODELING THE DISTRIBUTION OF BRINE AND SALT IN AN ICE SHELL.

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Introduction: The presence of liquid water has long guided the search for life beyond Earth. Once thought to be confined to the “Goldilocks zone”, vast saltwater oceans have been inferred to exist beneath the thick ice shells of moons in the Jovian and Saturnian systems [1]. Although these sub-ice oceans represent the most compelling potential habitats in the outer solar system, their overlying ice shells pose a challenge to life detection missions aiming to directly sample them.

Salts entrained from the ocean during the formation and thickening of these ice shells would allow liquid water to remain stable within the ice shell interior as brine well below the pure ice pressure-melting temperature. These brine pockets could represent an oasis for life trapped within the ice and serve as a more accessible target for future missions. Furthermore, the volume fraction of brine, solid salt, and ice in the ice shell governs bulk thermophysical properties (e.g., density, thermal conductivity, specific heat capacity, viscosity), which modulate processes of surface-ice-ocean exchange, as well as dielectric properties (e.g., electrical conductivity, relative permittivity), which influence signal reflection and attenuation for future ice-penetrating radar and electromagnetic investigations. As such, development of a modeling framework for the distribution of brine and solid salts in impure water ice represents a crucial step in the search for and characterization of potential habitats beyond Earth.

Methods: We present a framework for modeling the volume fraction of ice, brine, and solid salts in an ice shell of bulk salinity, S , inspired by models developed for terrestrial sea ice [2]. Whereas previous methods have used experiments to obtain properties of the solution as a function of temperature, we employ the opensource aqueous geochemistry program FREZCHEM which supports the extension of this approach to impure water ice of any composition [3].

Impure ice is a multiphase, multicomponent system made up of solid ice, solid salts, liquid water, dissolved salts (ions), and trapped gases. The amount of brine stable in ice is governed by the bulk salinity of the ice, the temperature, and the composition of the salts. Through knowledge of the solution properties as a function of temperature (e.g., brine density, brine salinity, relative amounts of salt in brine vs. solid salt),

the brine volume fraction as a function of bulk ice salinity and temperature can be obtained. These properties are defined for a particular solution composition as a function of temperature between the pure ice pressure-melting temperature (0 °C for 1 atm) and the eutectic temperature. As such, only a single FREZCHEM simulation for a relatively dilute solution of a given composition across the relevant temperature domain is necessary to derive the phase behavior functions (Fig. 1). Note that we model equilibrium crystallization and as such the bulk composition of the system does not change. At temperatures below the eutectic, where brine is not thermodynamically stable, the volume fraction of solid salt is a simple function of the mass fraction and density of salt and pure ice. The pure ice density is modeled using the Gibbs potential function released by the International Association for the Properties of Water and Steam (IAPWS).

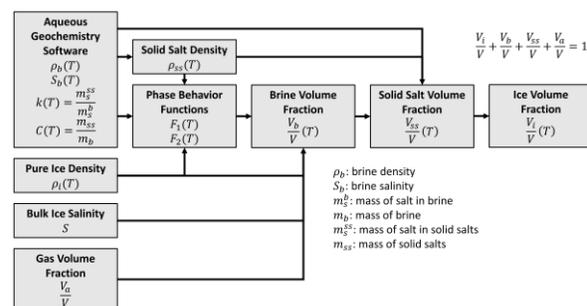


Figure 1. Framework for modeling the volume fraction of ice, brine, and solid salts.

We validate our proposed framework using terrestrial sea ice, with a composition represented by standard mean ocean water [4]. Figure 2 presents a comparison of the brine volume fraction estimated for sea ice using our model and the contemporary standard [5]. The models agree with each other across their defined domains, although our model predicts a slightly lower brine volume fraction at temperatures below -22.9 °C, where hydrohalite begins to precipitate. Both models are consistent with the “rule of fives”, which states that at a bulk salinity of 5 ppt, the brine volume fraction of sea ice is 5% at -5 °C [6]. Two notable limitations of [5] are: (i) the data used to derive the model phase behavior reflects a non-equilibrium freezing pathway for seawater (Ringer-

Nelson-Thompson) [7] and (ii) the model is not defined below $-30\text{ }^{\circ}\text{C}$. Our model reflects the equilibrium freezing pathway for seawater (Gitterman) and extends to the predicted eutectic temperature of $-36.2\text{ }^{\circ}\text{C}$ [8].

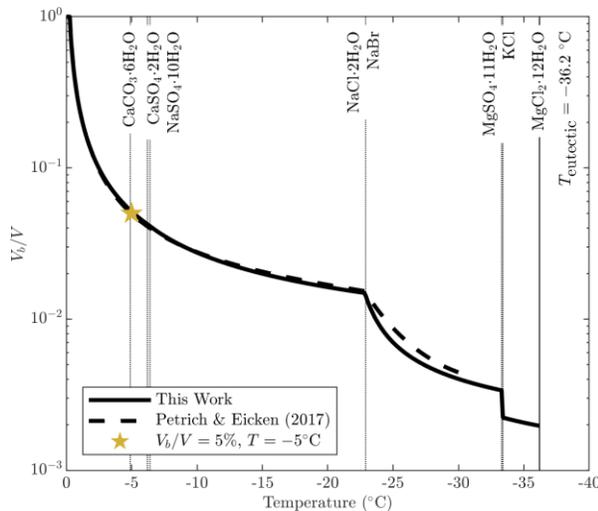


Figure 2. Validation of our brine volume fraction model for sea ice of 5 ppt bulk salinity, neglecting the presence of gases. The solid line represents our model derived using FREZCHEM v13.3 whereas the dashed line represents the model of [5].

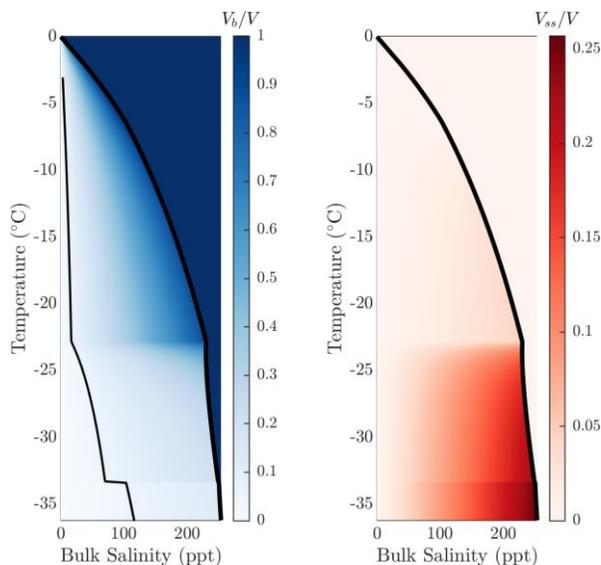


Figure 3. Brine (V_b/V) and solid salt (V_{ss}/V) volume fraction for sea ice. The thick black line depicts the liquidus and the thin black line depicts where the brine volume fraction is 5%, corresponding to an apparent percolation threshold in columnar sea ice [6].

Figure 3 illustrates the brine and solid salt volume fractions for terrestrial sea ice over a temperature range spanning from the pressure-melting temperature to the eutectic temperature and a bulk salinity range spanning from pure water to the eutectic composition.

A limitation of the proposed approach is that the pressure is assumed to be fixed (i.e., the pressure dependence of phase behavior is not modeled). This is not an appropriate assumption for modeling the stability of brine where ice shells exceed a certain thickness, and the influence of overburden pressure is no longer negligible. One atmosphere of pressure corresponds to ~ 100 meters of ice at Europa, which could represent $<1\%$ of the potential ice shell thickness. To account for the influence of pressure, multiple FREZCHEM runs over a range of pressures are needed to obtain surfaces, as opposed to curves, for the phase behavior functions.

Discussion: We will apply our proposed framework to Europa’s ice shell. We will prescribe a bulk composition based on spectroscopic observations of the surface which suggest Na, Cl, Mg, and SO_4 are likely the dominant impurities [9]. We will consider binary end-member cases for bulk ice shell composition (e.g., NaCl, MgSO_4) before exploring permutations of these species to represent more complex sulfate-dominated and chloride-dominated systems. We will first assume a pressure of one atmosphere to model an ice shell of arbitrary thickness, then we will account for the influence of pressure to examine the vertical extent of brine for a range of ice shell thicknesses and an assumed temperature profile.

Because the presence of water alone is not sufficient to evaluate habitability, selected metrics will be used to further evaluate the distribution of potential habitats. The water activity, ionic strength, and SO_4/Cl ratio will be plotted for Earth seawater and the sulfate-dominated and chloride-dominated European ice shells to evaluate the suitability of these briny, in-ice environments as potential habitats. We evaluate Earth seawater as validation since sea ice represents a known in-ice habitat on Earth.

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