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SeaFreeze : A modular thermodynamic framework for modeling all solar system planetary hydrospheres, including ice polymorphs and aqueous solutions at high-pressures.

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Abstract

SeaFreeze is a new modular and open-source self-consistent thermodynamic representation for high-pressure solution chemistry and ices. It is implemented in Python, Matlab and Fortran. It is based on new accurate in-situ sound speed and X-Ray diffraction data for both aqueous fluids and high pressure ice polymorphs. It is able to derive major equilibrium thermodynamic properties for each phase (e.g. density, bulk modulus, heat capacity, thermal expansivity, chemical potential, entropy) and predict their stability. The gamut of applications covers the entire range of possible conditions found in hydrospheres and oceans in our solar system (200-400K, 0-2.3GPa).

1. Introduction

Hydrospheres of water-rich planetary bodies (e.g. Enceladus, Europa, Ganymede, Titan, ocean exoplanets, etc.) are currently considered the most likely places where deep liquid water environments could currently exist, making them prime targets for the search of extraterrestrial life in our solar system and beyond. Their hydrospheres could include thick liquid oceans with solutes such as Na, Cl, Mg, SO_4, CH_4, CO_2, etc. For the largest planetary bodies like Ganymede, Callisto and Titan, a high pressure ice mantle, possibly composed of ice III, V, VI and eutectic phases (e.g. salt hydrates), is expected between the ocean and the silicate core. Precise knowledge of elastic and thermal properties of these phases as a function of P and T is therefore essential to the modeling of the geological structure and evolution of planetary hydrospheres. Surprisingly, if many thermodynamic descriptions exist for aqueous solutions up to 100MPa, no self-consistent framework can accurately represent all equilibrium properties at pressures relevant for icy worlds interiors (100-10,000 MPa). This is mainly due to the lack of experimental data in that range of thermodynamic conditions. We present here a new Gibbs energy thermodynamic framework named SeaFreeze based on new accurate experimental data and a fundamental and robust physical model. This enables one to derive equilibrium thermodynamic properties at any pressure-temperature-composition coordinates relevant to solar system hydrospheres.

2. Methods

New, accurate experimental data were acquired at temperatures and pressures appropriate to the modeling of hydrospheres. X-ray diffraction was used to investigate high-pressure ices and hydrates. Sound speeds were obtained with an accuracy of 0.02% up to 700MPa, using ultrasonic measurements, and to higher pressures in the diamond-anvil cell with 0.2% accuracy using Impulsive Stimulated Scattering. The data were used to derived a Gibbs energy surface for each phase, using standardized local basis functions[1].

3 Results and implications

This Gibbs representation for stable solids phases (ice Ih, III, V, VI) and aqueous solutions H_2O-(Na,Cl,Mg,SO_4), available as open source function in Matlab^{TM}, FORTRAN and Python languages, can provide self-consistent equilibrium thermodynamic properties (Gibbs energy P-T-X derivatives) inlcuding entropy, density, chemical potential, bulk modulus, heat capacity and thermal expansivity. Furthermore this framework was developed to be modular, so new solution chemistry and solid phases can be added seamlessly without any edits to the core of the representation. From this new comprehensive representation, one can can explore equilibrium properties inside all conditions present in solar system planetary hydrospheres (200-400K 0-2.3GPa and e.g. 0-5 molal for NaCl solute). Some of the remarkable outcomes of our study are :

- Solute driven melting point depression (Fig.1) and density inversions (Fig.2) between high-pressure ices and (Na,Cl,Mg,SO_4) salt solutions can be accurately predicted for ice Ih, III, V and VI.
- Melting point depression of ice III allows ice II to be stable in equilibrium with the fluid starting at 2 mol·kg^{-1} of dissolved NaCl.
- Depending on the type of solutes, the thermal gradient inside planetary hydrosphere can radically change. Presence of anti-freeze solutes does not necessarily translate in thinner high pressure ice mantle and deeper oceans.
- Eutectic point composition varies significantly with pressure, as well as with the phases present at the eutectic, which could strongly influence the geodynamics of the high pressure mantle.

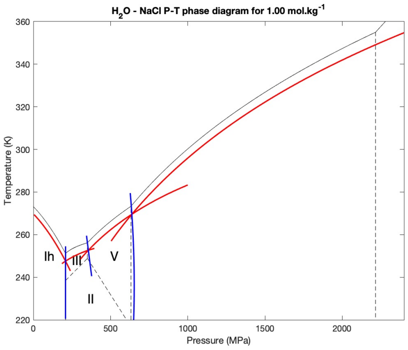

Figure 1: Predicted phase diagram from the new representation for 1 molal NaCl. Pure water melting curve as a lack line, 1 molal NaCl melting curve as red line. Blue line represent predicted solid solid phase transition based on thermodynamic modeling. dashed black line represent solid-solid phase transition from experimental measurments [2].

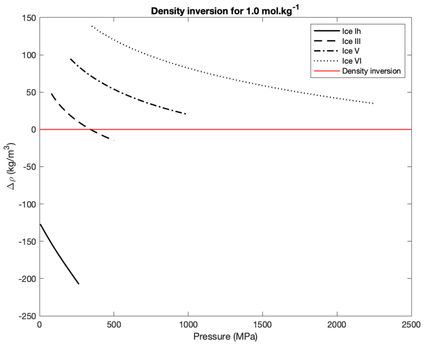

Figure 2: Predicted density inversion along the melting curves from the new representation for 1 molal NaCl and all ice polymorphs. Here ice Ih and ice III over 400MPa becomes less dense than the NaCl brine.

4. Summary and Conclusions

We developed a new self-consistent and modular thermodynamic representation for H_2O-rich chemistries that allows fast computation of thermodynamic properties in the pressure-temperature-composition range of interest for potentially habitable hydrospheres of icy moons and water-rich exoplanets. The main framework will be presented, as well as examples of thermodynamic property predictions (matching experimental data at high pressures), and implications for the interiors of water-rich planetary bodies.

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