



Contribution ID: 40

Type: Poster

Liquid-like layers on ice in the environment: bridging the quasi-liquid and brine layer paradigms

Monday, 6 June 2011 12:05 (1h 10m)

Liquid-like layers on ice significantly influence atmospheric chemistry in polar regions. In the absence of impurities a nanoscale region of surface disorder known as the “quasi-liquid layer”(QLL) may exist at temperatures well below the bulk melting point (down to $\sim -30^{\circ}\text{C}$). Surface and bulk impurities are known to modulate the QLL thickness. In aqueous systems containing ionic solutes a liquid brine layer (BL) may form upon freezing due to the exclusion of impurities from the ice crystal lattice coupled with freezing point depression in the concentrated surface layer. Brine layers are conceptually distinct from the QLL, which can exist in the absence of impurities.

We have developed a unified model for liquid-like layers in environmental ice systems that is valid over a wide range of temperatures and solute concentrations, spanning the QLL and BL regimes. The model consists of two coupled modules describing the thickness of the BL and the QLL. The BL module is derived from fundamental equilibrium thermodynamics, whereas the QLL formulation is derived semi-empirically based on statistical mechanical principles and previously published QLL thickness data. The resulting unified model has been tested against experimental data from literature and applied to several environmentally important systems, such as $\text{HCl}(\text{g})$ -ice, $\text{HNO}_3(\text{g})$ -ice, and frozen sea ice. This model can be used to improve the representation of air-ice chemical interactions in polar atmospheric chemistry models.

Please list some keywords

QLL brine modeling

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Session Classification: Lunch and Poster