Geophysical Research Abstracts,
Vol. 11, EGU2009-549, 2009
EGU General Assembly 2009

Adsorption of small, partially oxidized hydrocarbons at the surface of ice, as seen by Grand Canonical Monte Carlo simulations

G. Hantal (1,2), P. Jedlovszky (1), L.B. Partay (1), P.N.M. Hoang (2), and S. Picaud (2)

(1) Laboratory of Interfaces and Nanosized Systems, Institute of Chemistry, ELTE University, H-1117 Budapest, Hungary (hantal@elte.hu), (2) Institut UTINAM-UMR CNRS 6213, Université de Franche-Comté, F-25030 Besançon Cedex, France

The adsorption isotherm of various partially oxidized methane derivatives, such as methanol, formaldehyde, formic acid and acetone on ice has been determined at 200 K by using the Grand Canonical Monte Carlo computer simulation method. The results are compared in detail with available experimental data. The experimental and simulated isotherms of methanol agree well with each other, their deviations can be explained by a small (about 5 K) temperature shift in the simulation data and, possibly, by the non-ideality of the ice surface in the experimental situation. In a clear contrast with other partially oxidized small hydrocarbons, the obtained isotherm of formaldehyde does not show any particular stability of the saturated adsorption monolayer of the molecules, again in accordance with experimental observations. Further, in contrast with that of the other adsorbates considered, the obtained adsorption isotherm of formaldehyde can be well described with the functional form of the Langmuir isotherm, indicating the relative weakness of the lateral interactions between the adsorbed molecules in this system.

The main thermodynamic driving force of the adsorption is found to be the possibility of the formation of water-adsorbate hydrogen bonds in every case. However, while methanol, acetone and formic acid molecules can form multiple hydrogen bonds with the ice phase, an adsorbed formaldehyde molecule has never been found to form more than one hydrogen bond with the surface waters. Also, the lateral interaction of the adsorbed molecules is found to be considerably weaker in the case of formaldehyde than in the case of the other three adsorbates, which are able to form also lateral hydrogen bonds or strong dipole-dipole complexes.