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Kinetics of the CO_2 hydrate formation and decomposition at Martian conditions – in-situ neutron diffraction and shrinking core modeling

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Formation (and decomposition) of gas hydrates is a process not well understood at present despite its major importance for geological/planetological and technological processes. A number of competing phenomenological models have been proposed but still an exact physico-chemical model does not exist. Due to the lack of experimental data a check of the existing models is impossible in any detail. Here we give our contribution to the filling of this gap, presenting results from our neutron diffraction experiments on CO_2 hydrate formation and decomposition. Neutron diffraction is the only method available at present to measure the hydrate transformation rates in-situ. The good time resolution in following the fast initially transforming ice/hydrate system is of crucial importance. The last goes hand in hand with the need for high neutron flux at the position of the sample. Moreover, the good resolution in 2θ is a must for the precise estimating of the transformation at any time during the reaction. The high flux at the sample position, the large stationary position sensitive detector and the fast data acquisition system make D20 at ILL, Grenoble an ideal tool for studying gas hydrate kinetics. The large pressure-temperature region of interest for hydrate formation and decomposition and the strong sensitivity of the kinetics on the temperature changes require the implementation of sophisticated vacuum- and high-pressure equipment, discussed here, as well as a precise temperature control. The latter is provided by the Helium Flow Cryostat on D20. The high time resolution requirement results in a large set of diffraction pattern files per single reaction that runs for a day usually. Therefore, an automatic procedure for processing large number of patterns is conversed and implemented. During this automatic loop, every single file of the set is analyzed using the full-pattern Rietveld refinement software GSAS. The data processing yields the

fraction of ice, transformed into hydrate with a statistical precision of 1.4 – 2 % for 5 min time intervals. Analyses of the different reactions using different models are also shown.