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Predicted occupancies in gas hydrates on Titan and Mars: sensitivity on treatment of intermolecular interactions.

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We investigate here the sensitivity of gas hydrate occupancies predicted on the basis of van der Waals-Platteeuw theory, as a function of the treatment of the intermolecular guest-water interaction potential. First, we determine the minimum number of water molecules that have to be taken into account in the calculations of this interaction potential. We show that analytical correction terms that account for the interactions with the water molecules beyond the cutoff distance (typically chosen to take into account at least 4 water layers around the guest molecule) must be introduced to improve significantly the convergence rate, and hence the efficiency of the computation of the Langmuir constants. Then we use different recent guest-water interaction potential models to calculate the cage occupancies in pure methane or carbon dioxide clathrates. We show that the corresponding predicted cage occupancies can vary significantly depending on the model, although all the results are within the uncertainties of the available experimental data. That sensitivity becomes especially strong in the case of multiple guest clathrates, and, for instance, the results obtained for guest clathrate hydrates potentially formed on the surface of Mars can vary by more than two orders of magnitude depending on the model. These results underline the strong need for experimental data on pure and multiple guest clathrate hydrates, in particular in the temperature and pressure range that are relevant in extreme environment conditions, to discriminate among the theoretical models.