

Kinetic parameters of pelagic nitrifying communities: consequences on nitrite dynamics in the Seine River downstream of Paris

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Elevated nitrite concentrations are observed in the Seine River downstream of Paris and its main waste water treatment plants (WWTP). In order to understand the persistence of nitrite in the Seine, we determined kinetic parameters of pelagic ammonia- and nitrite-oxidizing communities. *In situ* ammonia- and nitrite-oxidation rates were deduced by determination of the kinetic parameters of the two processes combined with modeling. We compared the *in situ* rates and kinetic parameters upstream and downstream of the WWTPs during different seasons. The results showed both spatial and temporal variations of the *in situ* nitrification rates and kinetic parameters (e.g., maximal oxidation rate, half-saturation constant). At each given site and season, the *in situ* ammonia- and nitrite-oxidation rates were however similar, most likely resulting in little changes in water column nitrite concentrations. The results confirm that the elevated nitrite concentrations monitored in the Seine River are due to high nitrite released by the WWTP. In addition, the low nitrification rates and the equilibrium between ammonia- and nitrite-oxidation rates appear to prevent the elimination of nitrite from the system, leading to its persistence over more than 100 kilometers. The spatial and temporal variations of kinetic parameters reflect the dynamic microbial community structure and activity and may have implications on biogeochemical models.

Computer simulations of carbonates in water

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Over the last thirty years a lot of effort has been made to understand the structural, surface and crystal growth properties of carbonates in aqueous environments, both experimentally and computationally. The ever increasing resolution of experimental techniques and power of supercomputer are rapidly closing the gap between what the two approaches can achieve. Arguably calcium carbonate is among the most studied minerals, but while there is a general consensus that its crystalline phases grow via an amorphous precursor, there is still much debate about the existence of pre-nucleation clusters and whether the nucleation follows a classical or non-classical pathway. Moreover, other carbonates are comparatively less studied and less understood.

Here we will present a recent force field developed to reproduce the thermodynamic properties of the alkaline-earth carbonates X-CO₃ (X=Mg, Ca, Sr and Ba). This force field is used to study the different stages of the crystallisation mechanism, from isolated ions in solution to pre-nucleation clusters, nanoparticles and the growth of fully developed crystals. These studies include the calculation of reaction free energies (Figure 1), IR spectra and both structural and dynamical properties, and they demonstrate that carefully developed computational models are capable of quantitatively reproducing experimental observations.

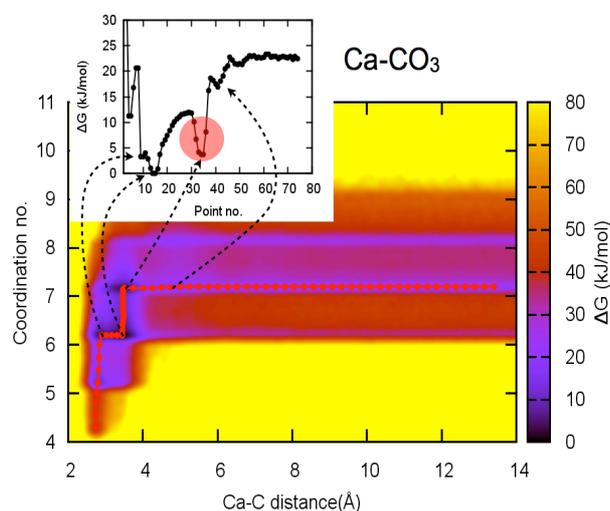


Figure 1 Ca-CO₃ pairing free energy calculated using the metadynamics technique with 2 collective variables.