



Mechanism of amorphous silica particles precipitation: simulation approach compared to experimental results

Claudine NOGUERA (1), Bertrand FRITZ (2), and Alain CLEMENT (2)

(1) CNRS, INSP, UMR 7588, F-75252 Paris Cedex 05, France (claudine.noguera@insp.jussieu.fr), (2) Université de Strasbourg/EOST, CNRS, Laboratoire d'Hydrologie et Géochimie de Strasbourg, 1 rue Blessig, F-67084 Strasbourg Cedex, France(bfritz@unistra.fr)

Despite its importance in numerous industrial and natural processes, many unsolved questions remain regarding the mechanism of silica precipitation in aqueous solutions: order of the reaction, role of silica oligomers, existence of an induction time and characteristics of the particle population. Beyond empirical approaches used in the past, we demonstrate that the classical nucleation theory associated to a size dependent growth law, as embedded in the NANOKIN code (1-3), allows a quantitative description of precipitation occurring under largely different experimental conditions : preexisting initial supersaturation in a large domain of temperature (5-150°C) and chemical composition (4), supersaturation reached by neutralization of a high pH silica solution (5) or by fast cooling (6). In that way, the mechanism of silica precipitation can be unraveled. We are able to discard the hypothesis of an induction time as an explanation for the plateaus observed in the saturation curves in these experiments. We challenge the role of oligomer incorporation at the growth stage to account for the observed rate laws and we stress the difference between the order of the growth law and the order of the total reaction rate. We also demonstrate that the characteristics of the particle population are strongly dependent on the way supersaturation is reached (7). Such a microscopic approach thus proves to be well suited to elucidate the mechanism of nanoparticle formation in natural and industrial contexts, involving silica, but also other mineral phases produced as nanoparticles (8).

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