MODELLING EQUILIBRIUM DISTRIBUTION OF IONS AND MOLECULES IN A HETEROGENEOUS SYSTEM OF CaCO₃–WATER–GAS PHASE UNDER BOTH EQUILIBRIAL AND NON-EQUILIBRIAL CONDITIONS

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Abstract

In many places, including Northern Estonia, the soil bedrock is limestone, consisting mainly of *CaCO₃*. Equilibrium processes in aqueous medium involving dissolved *CO_2* and solid *$CaCO_3$* play a vital role in many biological and technological systems. In this study, a model for equilibrium distribution of ions and molecules in the ternary heterogeneous system solid CaCO₃–water–gas phase containing CO_2 under both equilibrial and non-equilibrial conditions was developed. The model can be used for the determination of concentrations of all components in the water phase over a wide range of concentrations of CO_2 in water, allowing the assessment of the impact of anthropogenic processes on the natural environment and could be usefully applied in water and wastewater technology. It can also be useful for developing innovative methods for the measurement of aqueous CO_2. As algae in water utilize dissolved *CO_2* in photosynthesis, it leads to an increase in pH and bacteria will produce *CO_2*, which, in turn, leads to a decrease in pH. Therefore the concentration of *CO_2* will vary in a large scale in the aqueous environment. The equilibrium concentrations of dissolved *CO_2* in the liquid phase at a given partial pressure of *CO_2* in the gaseous phase was calculated in the range of $p(CO_2)_G \cong (8.08\times10^{-7} \div 2.37\times10^4)$ ppm at 25 °C. Quantitative evaluation of the equilibrium distribution of ions and molecules in the system $CaCO_3$–CO_3^{2-}–HCO_3^-–H_2CO_3–CO_2 at an equilibrium with gas phase identified a relevant minimum solubility of $s[CaCO_3]_{min} \cong 0.1$ mmol/L. The model has been experimentally validated.

Keywords

Calcium carbonate, Carbon dioxide, Water, Equilibrium, Ternary system.