

A MODEL OF CLOSED EQUILIBRIUM SYSTEMS $\text{H}_2\text{O}-\text{CO}_2-\text{CaCO}_3-\text{NaH}_2\text{PO}_4$

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The aqueous systems containing carbonaceous and phosphorous species are present in many waste waters of various types and origin. Limestone bedrock, which consists mainly of CaCO_3 , affects waste- and reject water treatment. Variation in the concentration of dissolved carbon dioxide $[\text{CO}_2]_w$ causes changes in the solubility of CaCO_3 and pH in an equilibrium system. The system $\text{H}_2\text{O}-(\text{CO}_2)_w-\text{CaCO}_3$ was taken as the basis for modelling the closed system $\text{H}_2\text{O}-(\text{CO}_2)_w-\text{CaCO}_3-\text{NaH}_2\text{PO}_4$ [1]. The distribution of ions and molecules in the closed system $\text{H}_2\text{O}-(\text{CO}_2)_w-\text{CaCO}_3-\text{NaH}_2\text{PO}_4$ is described in terms of a structural scheme.

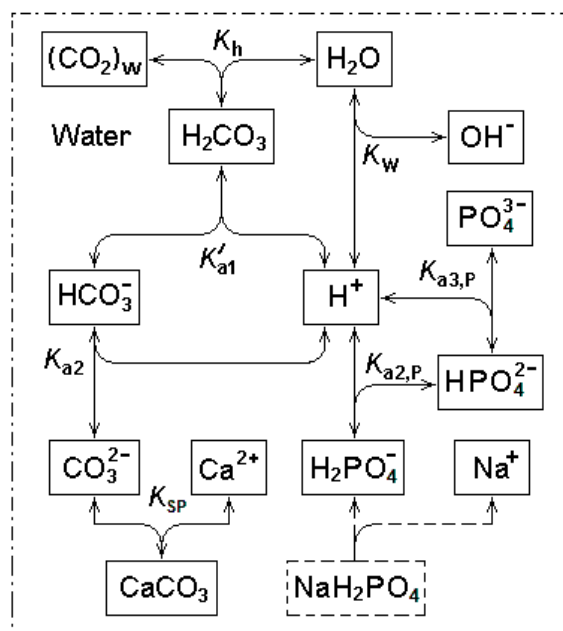


Fig.1 Structural scheme of the equilibrium distribution in the final closed system of $\text{H}_2\text{O}-[\text{CO}_2]_w-\text{CaCO}_3-\text{NaH}_2\text{PO}_4$, where K_h is the hydration constant of CO_2 , K_{a1} the true acid dissociation constant of H_2CO_3 , K_{a2} the acid dissociation constant of HCO_3^- , K_{sp} is the solubility product constant of CaCO_3 , K_w the ion-product constant of water, and $K_{a2,p}$ the dissociation constant of H_2PO_4^- ions, $K_{a3,p}$ the dissociation constant of HPO_4^{2-} .

The developed model of the equilibrium closed system $\text{H}_2\text{O}-(\text{CO}_2)_w-\text{CaCO}_3-\text{NaH}_2\text{PO}_4$ can be used to determine concentrations of all components in the water phase over a wide range of natural and industrial conditions. The model allows one to assess the impact of anthropogenic processes on the environment and could be applied by environmental technologists in water and wastewater treatment.

References

1. Tenno, T., Uiga, K., Mashirin, A., Zekker, I., and Rikmann, E. Modelling closed equilibrium systems of H_2O -dissolved CO_2 -solid CaCO_3 . *J. Phys. Chem. A*, 2017, **121**, 3094–3100.