The method of definition of the effective thermodynamic parameters of trace metals sorbed forms in bottom sediments from sequential extraction data

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Application of thermodynamic modeling to forecast of trace metals migration in water ecosystems is difficult because bottom sediments composition in reservoirs is very changeable and uncertain. We offer the alternative approach for solving similar problems. It is based on use of empirical information about distribution of mobile and potentially mobile forms of trace elements. Such type of information can be received using sequential extraction scheme (for example Tessier scheme). Effective thermodynamic parameters for certain object are calculated from this data.

System «pore water – solid phase» of bottom sediments is considered as multicomponent system in thermodynamic model. It includes aqueous phase, individual solid phases and principal sorbing phases (clay minerals, iron and manganese hydroxides and organic matter) assumed as ideal solid solutions.

The coefficients of trace metals selectivity with respect to calcium for the main sorbed forms were calculated based on the results of the analysis of extracts from the solid phase of bottom sediments and pressed pore waters. Based on these coefficients, the imaginary increments of the Gibbs free energy $\Delta g°(T)$ for the sorbed forms were calculated. The quantity $\Delta g°(T)_{CaX}=0$ was taken as a reference point of the imaginary $\Delta g°$.

We performed the calculation of metal distribution between sorbents and pore solution using the calculated effective thermodynamic parameters. The thermodynamic calculations accurately reproduce the empirically obtained trace metals distribution in bottom sediments.