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Thermodynamic modeling of underground water chemical composition and model R/W parameter

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Approach to the use of the model R/W (rock/water mass ratio) of the thermodynamic computer HCh program (Yu.V.Svarov) in the forecasting of the underground water hydrochemical type was developed. Principle of the realization of this approach is demonstrated in the Figure.

If volume of 1 kg of the rock and its porosity (n_s) are known, volume (V_s) of the porous space can be determined. Multiplying porous space volume (V_w) by the density of the solution (ρ_w) which is filtering through rock sample we can obtain R/W value.

Water-rock system is considered. Water moves through the porous space. Filtering capacity of the rocks primarily depends on the peculiarities of the porous space. Size of the particles in its turn determines value of the porous space. Values of density (ρ, g/cm^3) to porosity (n, %) of water retaining rocks are following: clay ρ=1.6-2.9, n=20-40; sandstone ρ=2.6, n = (10-12)-20.; limestone ρ=2.12-2.8. n=5; dolomite ρ=2.8-2.99, n=5.

Using these data dependence of number of the cycles of water exchange for a give rock type depending on R/W ration can be obtained.

Equilibrium compositions of aqueous phase in carbonate rocks – water system for different R/W rations were obtained in the course of thermodynamic modeling using HCh program complex (B.N. Ryzhenko, S.R. Krainov, 2003). Using these data and our

approach we could estimate to a first approximation number of cycles of the complete replacement of water in the water-rock system and determined corresponding water type.

It turned out that in the carbonate rock – water system chloride-sulfate sodium-calcium type of aqueous phase arises if R/W ration is less than unity and number of water exchange cycles is more than 40.

We suggest the following algorithm to be used to obtain standard dependences hydrochemical underground water types on R/W ratios:

1. Choice of the system of the elements: Ca, Mg, Na, K, S, C, Cl, O_2, H_2;
2. Selection of main rock-forming minerals containing the chosen elements;
3. Schematization of the hydro geological processes of the formation of hydro geological structures and determination of system-forming parameters (temperature, pressure, openness or closeness of the system, presence of gases etc);
4. Thermodynamic modeling of the water-rock system, the rock consisting of the minerals chosen on the 2^{nd}stage;
5. Presentation of the solution mineralization obtained in the course of modeling via velocity of the solving of the chosen minerals and determination of the time of formation of the water – rock system;
6. Transition from the time to the model R/W parameter via number of water exchange cycles;
7. Conversion of the mineralization into hydrochemical underground water type and finding of corresponding W/R value.