Groundwater in the overburden of the Upper Silesian Coal Basin

Krzysztof Labus_a), Arnošt Grmela_{b)c}), Nad'a Rapantová_b)

 ^{a)}Silesian University of Technology, Institute for Applied Geology, 44-100 Gliwice, 2 Akademicka St, Poland; krzysztof.labus@polsl.pl tel. +48 32 2372942
^{b)}VŠB –Technical University Ostrava, HGF, IGI,17.listopadu 15, Ostrava–Poruba,708 33 Czech Republic,

nada.rapantova@vsb.cz_tel. +420 596993501, arnost.grmela@vsb.cz_+420 595663500 ^{c)} ATH, Inst.WNMiŚ, Bielsko-Biała, Poland;

Abstract

This work was aimed at modeling the hydrochemical evolution of groundwaters in overburden of the Czech part of the USCB. Inverse modeling allowed the qualitative definition of hydrochemical reactions able to control the groundwater chemistry. The consequent one-dimensional advective-dispersive-reactive transport model of water-rock interactions within the aquifer, corroborated predictions, that the recent composition is influenced by infiltration of rainwater, diluting sedimentary waters of marine origin in presence of geogenic CO_2 .

Key words: the Upper Silesian Coal Basin, geochemical modeling, mine water, Miocene seawater

Introduction

Waters from the overburden of Carboniferous productive formation are considered as a major hazard to mining activity within the Czech part of The Upper Silesian Coal Basin (USCB). They may be derived from Miocene seawater (from the Skawina formation and the coarse clastic Lower Badenian aquifer Dębowiec formation = "detrit") mixed with water types of another origin (waters from the carboniferous massif, waters from the deeper parts of the rock massif and respectively from the recent infiltration quaternary waters). Mining drainage, reaching the depth of 1200 m, caused partial depletion of the groundwater resources, and in consequence led to changes of their chemical composition.

Modeling groundwater chemistry of Lower Badenian aquifer

Inverse modeling by means of PHREEQC (Parkhurst and Appelo 1999) was applied aiming the qualitative definition of hydrochemical reactions that may have been controlling the groundwater evolution along their flowpath through the Lower Badenian aquifer. It was assumed that the primary fluid filling aquifer pore space was the sedimentary water of the composition equal to the seawater, while the composition of the resulting fluid is the one of representative sample taken from a well testing the Lower Badenian aquifer (Tab. 1). Mineral phases of the reactions were chosen on the bases of archival logs (Pišta 1961, Hufová 1971, Květ 1980) as well as on petrographic analyses of drill cores.

The calculations allowed formulation of several models describing the processes of forming groundwater chemistry in effect of primary pore fluid dilution by infiltrating precipitation waters, accompanied by: CO_2 inflow, ion exchange and dissolution of carbonates and/or alumosilicates (examples are presented in the Tab. 1).

Results of simulated reaction of primary fluid (seawater) with phases that were identified by means of inverse modeling (Model I - Tab. 1) are presented in the Fig. 1. The simulation was performed according to the "flow-through" procedure which minerals are prevented from dissolving once they precipitate. This option is helpful for modeling chemistry evolution of a packet of fluid as it migrates through an aquifer. Once minerals form, they are isolated from the packet so that they can not backreact with the fluid should they become undersaturated farther along the flow path (Bethke 1996). This reflects the situation of a fluid which looses the contact with phases precipitating as it migrates within the aquifer.

Table 1 Chemical composition of fluids - end-members in the inverse modeling of the LowerBadenian groundwater's chemistry, and the reaction phases identified

parameter	Seawater (after Nordstrom et al., 1979) primary fluid [mol/kg] F _p	Sample 109 – resulting fluid [mol/kg] F _k	product	Model I [mol] $F_p/F_k=$ 5,043.10 ⁻²	Model II [mol] $F_p/F_k=$ 5,043 $\cdot 10^{-2}$	
			Dissolution			
Temp	20	10	$CO_2(g)$	4,276·10 ⁻²	7,693·10 ⁻²	
pН	8,22	7,6	H ₂ O	$5,275 \cdot 10^{+1}$	$5,282 \cdot 10^{+1}$	
pe	8,451	-	Calcite	3,418·10 ⁻²	9,118·10 ⁻⁴	
Ca ²⁺	$1,066 \cdot 10^{-2}$	7,930.10-4	Dolomite	$3,270 \cdot 10^{-3}$	$3,270 \cdot 10^{-3}$	
Mg ²⁺	5,505·10 ⁻²	6,187·10 ⁻³	NaX	7,436·10 ⁻²	$4,365 \cdot 10^{-2}$	
Na ⁺	4,852·10 ⁻¹	$1,052 \cdot 10^{-1}$	Plagioclase	-	$4,953 \cdot 10^{-2}$	
			Precipitation			
Cl	5,655.10-1	$2,826 \cdot 10^{-2}$	Chalcedony	-	$-6,1420\cdot10^{-2}$	
SO4 ²⁻	2,925.10-2	-	CaX ₂	$-3,718\cdot10^{-2}$	$-2,182 \cdot 10^{-2}$	
HCO ₃ ⁻	2,411.10-3	$7,550 \cdot 10^{-2}$	Kaolinite	-	$-3,418\cdot10^{-2}$	

Figure 1 Dependence of pH, and selected ions concentration on the degree of the reaction progress (Rxn) of the primary fluid (seawater) with the phases identified by the reverse modeling (Model I - Tab. 1)



Figure 2 Primary regime of fluids migration into the Dębowiec formation aquifer in the Czech part of the USCB



Results of the inverse modeling gave also a basis for one-dimensional advective-dispersive-reactive transport model of water-rock interactions within the aquifer of the Dębowiec formation. The model was formulated assuming that the rainwater (composition after Cornell 1996 vide Hiscock 2005) evaporated by 70% infiltrates the aquifer and dilutes pore water (of seawater composition after Nordstrom et al. 1979) in presence of geogenic CO_2 (Fig. 2).

The model was prepared with use of the PHREEQC code. The following assumptions regarding the petrophysical characteristics of Lower Badenian sediments were made: bulk density (ρ_b) - 2,2 g/cm³; total porosity (n) - 0,15; effective porosity (n_e) - 0,1; weight contents: carbonates 25%., clay minerals 17% (after Hufová 1971) and 0,5% C_{org}, skeletal density (ρ_s) - 2,6 g/cm³, rock mass per volume of effective porosity (ρ_{be}) - 2,364 g/cm³. As the rock mass per 11 of effective pores is 23,364 kg - 5,91 kg of carbonate minerals is associated with the unitary volume of pore space. If the carbonates were formed solely by calcite or dolomite, their mass should equal to 59 mol of CaCO₃ or 32,07 mol CaMg(CO₃)₂ respectively. The cation exchange capacity (CEC=14 mval/100 g) was calculated after the following formula (Appelo and Postma 1993):

CEC [mval/100 g] = $0.7 \cdot (\% \text{ mass clay minerals}) + 3.5 \cdot (\% \text{ mass. } C_{\text{org}})$.

The obtained CEC value is equal to $3,3\cdot10^3$ mval/dm³ (for the rock mass corresponding with 1 dm³ of effective pore space). Proportion between the cell length (L) and the dispersivity (α) was accepted as L: $\alpha = 10:1$, diffusion coefficient D = $1\cdot10^{-9}$ ms⁻¹.

Reactions take place in a column consisting of 20 cells filled with seawater (Fig. 3). The fluid is in equilibrium with exchanger, containing 165 mval $(3,3\cdot10^3/20 \text{ mval})$ ion exchange sites in each cell. Water reacts with calcite (20·0,1 mmol), dolomite (20·1,0 mmol) and CO₂ (20·2,25 mmol). First and the last cell are defined by the third type (Cauchy) boundary condition. Infiltrating rain water, evaporated by 70%, and equilibrated with calcite and dolomite enters the first cell. Concentrations are monitored in the resulting fluid when it is leaving the last cell.

Figure 3 Scheme of the applied model of forming the chemistry of the groundwater in the Lower Badenian sediments



Figure 4 Diagram of selected constituents of waters considered $[mg/dm^3]$, showing water type transformations - the modeling results



Modeling results give evidence (Fig. 4) that chemical composition analogous to the one of recent groundwater in the Lower Badenian sediments is reached when the 1.2 pore volumes of primary fluid are moved through the column. (composition of the representative sample is precisely reproduced). Calculations performed on the consecutive modeling stages, allowed to calculate compositions of theoretical fluids chemistry of which is consistent with groundwater chemistry ascertained within the aquifer (Grmela et al. 2004). The transformations of groundwater chemistry could presented in stages according to the water type changes, connected with the flow of water through the pore space (Tab. 2).

Table 2 Stages of the water type transformations due to the water flow through the pore space

Pore volumes exchanged	0,00-0,98	0,98-1,10	1,10-1,20	1,20-1,25	1,25-1,75	1,75
Water type	Cl-Na	Na-Cl-HCO ₃	Na-HCO ₃ -Cl	Na-HCO ₃	HCO ₃ -Na	HCO ₃ -Na-Mg

Conclusions

Groundwaters' evolution in overburden of the Czech part of the USCB was reconstructed by means of hydrochemical modeling. Applied procedures consisted of inverse modeling - qualitative definition of hydrochemical reactions potentially controlling the groundwater chemistry, and one-dimensional reactive transport simulation of water-rock interactions within the aquifer. According to the simulation results, the composition of recent groundwater in the Lower Badenian sediments is reached, when the 1.2 pore volumes of primary, sedimentary fluid are moved through the profile. The reactions proceed in presence of geogenic CO₂, and groundwater movement is possibly caused by rainwater infiltration. Results of the study may be helpful in prediction the flooding hazard in coal mines of the USCB, planning groundwater exploitation for balneology, monitoring hydrochemical changes within the areas of mines in closure, and estimating the participation of different fluxes in the collective mine waters.

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