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CALIBRATION OF DUAL POROSITY GROUNDWATER FLOW AND CONTAMINANT TRANSPORT MODEL FOR SIMULATION OF CLEANING VP-9C SITE [*]

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Abstract. The contribution summarises the results of our research in field of the dynamics of groundwater flow with dual porosity. The dual porosity means the fact that in porous medium, pores are partly active and partly inactive. The inactive pores are filled with solution but the velocity of flow in pores is negligible compared with velocity in active pores. Transport of dissolved solids is considered by the next basic processes – advection and dispersion in active pores and diffusion exchange between active and inactive pores. Final modelling solution of transport mechanism is made by the FVM, by time-explicit scheme. Flow is calculated by the mixed-hybrid model. Finally, the application in real conditions of uranium deposit Stráž in the Czech Republic is presented. Turonian aquifer is considered as a drinking water source for large part of the Czech Republic. The part of the Turonian aquifer is partially polluted by chemical mining of uranium on deposit Stráž. The evaluation of possible future danger is the key question. The calibration of the model using data from cleaning test site VP-9C is presented.

Key words. simulation, groundwater flow, contaminant transport, dual porosity, model calibration

1. Introduction.

The area of the Stráž block in north part of Czech Republic is geologically divided into two overlaying aquifers, Cenomanian and upper laying Turonian, splitted by the low Turonian aquitard. In the Cenomanian aquifer the chemical mining of uranium on the Stráž deposit was performed. In spite of the aquitard the upper laying Turonian aquifer was also polluted by injected sulphuric acid. Such pollution is the potential environmental hazard for drinking water sources in large area of Stráž block. The pollution of the Turonian aquifer has character of isolated plums of contamination. The cleaning of the Turonian aquifer is one of the main tasks connected to the whole process of remediation of the former uranium-leaching site.

For the complex evaluation of remedial strategies the numerical models of groundwater flow and contaminant transport were developed and applied. The groundwater flow model is based on mixed-hybrid formulation of FEM, see [1], [2], [3] and [4]. The contaminant transport model is based on FVM, time-explicit scheme, see [2] and [3].

The evaluation of the experimental extraction of contaminated Turonian solutions showed some inconsistency between modelling and experimental results. For that reason the transport model was equipped with module of dual porosity. This improved transport model was calibrated using experimental data from testing VP-9C site.

2. Model of dual porosity.

2.1. Characteristics.

By “dual porosity” we express that soil matrix is divided into two pore structures, active and inactive, see [7] and [8]. The inactive pores are filled with solution but the velocity of flow in pores is negligible compared with velocity in active pores.

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Let us denote:
n_a – active porosity,
n_s– inactive porosity (s = "slow") and
n – total porosity ($n = n_a + n_s$).

The transport of the contaminants is driven by the following aspects: advection and dispersion in active pores and diffusion exchange between active and inactive pores. See the symbolic structure on fig. 1.

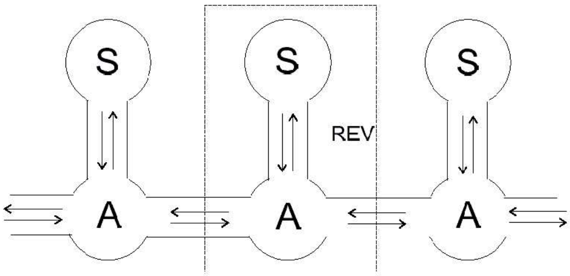


FIG. 1. *Model of structure of active (A) and inactive (S) pores*

2.2. Diffusion in pores. Further we focus only on the diffusion exchange between active and inactive pores. We expect that reader knows the problem of advection and dispersion in active pores, see [1], [2], [3].

Let us consider that diffusion flow between the volumes V_A and V_S is linearly dependent on difference of concentrations in these volumes with the proportion coefficient k

$$Q = k(c^l_A - c^l_S)$$

where Q is mass of the chemical component divided by time unit. The direct application of this formula in the model is not suitable. Numerical solution of parabolic equation in channel makes condition on time step even stronger then in advection case. For diffusion equation it must hold

$$\Delta t < \frac{(\Delta x)^2}{2b}$$

where b is diffusion rate. In such approach it would be necessary to split time step, which would dramatically slow the computations. The alternative is to use analytical solution of local exchange problem and its application for porous media. For time dependence of concentration of l-th substance in active and inactive pore volume, the following exponential forms

$$c^l_A(t) = (c^l_A(0) - \bar{c}^l(0))e^{k\frac{V_A+V_S}{V_A V_S}t} + \bar{c}^l(0)$$

$$c^l_S(t) = (c^l_S(0) - \bar{c}^l(0))e^{k\frac{V_A+V_S}{V_A V_S}t} + \bar{c}^l(0)$$

are valid for any time $t \in (0, +\infty)$ where $c^l_A(0)$ is concentration of the l-th substance in time $t = 0$ in active pore volume, $c^l_S(0)$ is concentration of the l-th substance in time

$t = 0$ in inactive pore volume and is average concentration of the l-th substance in time $t = 0$ in active and inactive volumes. The computing with use of exponential functions is not so slow and complicated as in the case of time step splitting. The coefficient k in the exponent includes the diffusion properties of the chemical components as well as the geometrical properties of the soil (characteristic length and cross-section of the pores). Expressing these properties we get

$$k\frac{V_A + V_S}{V_A V_S} = D^l \frac{Sn}{\lambda\lambda S n_S} = \frac{D^l n}{\lambda^2 n_S} = \alpha^l$$

where D^l denotes diffusivity of l-th substance, S is the cross-section of the pore (the area between active and inactive pore volumes), λ is the distance between both volumes. We defined notation $\alpha^l$for coefficient of substance mass exchange between the volumes. It can be written in the form $\alpha^l = D^l \times K_r$ where D^l depends only on chemical substance and K_r is depended on the properties of the soil.

In practice it is problematic to determine the mentioned local material characteristics (α^l, D^l, K_r) that in addition do not directly express the rate of exchange. For calibration of the model it is suitable to define following value

$$T^l_{1/2} = \frac{\ln 2}{\alpha^l},$$

which we call half-time of diffusion exchange. During this time the concentration changes from its initial value to the value

$$\frac{c^l_A(0) + \bar{c}^l(0)}{2}$$

which expresses that just a half of total mass possible for diffusion has already diffused. The model is implemented with the function

$$e^{-\frac{t}{T_{1/2}}\ln 2}$$

and the half-time of exchange $T_{1/2}$ is used as an input value instead of the diffusion coefficient.

2.3. Model implementation. The advective transport of contaminants is solved by explicit-in-time discretisation of FVM. The concentrations are considered in the elements of the mesh. Specific flows of the solution across the faces of the elements are calculated by mix-hybrid groundwater flow model. Explicit scheme time steps must reflect the CFL condition.

Appropriate soil properties have to be specified in the elements of the mesh. The properties are following: hydraulic conductivity, active and inactive porosity, diffusion coefficient dependent on the soil characteristics and diffusion coefficient dependent on the dissolved chemical component. The diffusion coefficients are set into the model in the form of half-time of exchange $T_{1/2}$. In this case it is hard to distinguish between values for soil and for each chemical component. Therefore the relative coefficient β^l is used for l-th chemical component. For the most important contaminant is $\beta^l = 1$.

3. Application of model on VP-9C site.

3.1. Model mesh. The model mesh covers the areas of three leaching fields VP-9A, VP-9B and VP-9C. The total model area occupies 1,3 km^2. The mesh consists of 1003 multielements that are vertically divided into 12 layers. The location and the shape of the mesh is on the fig. 2.

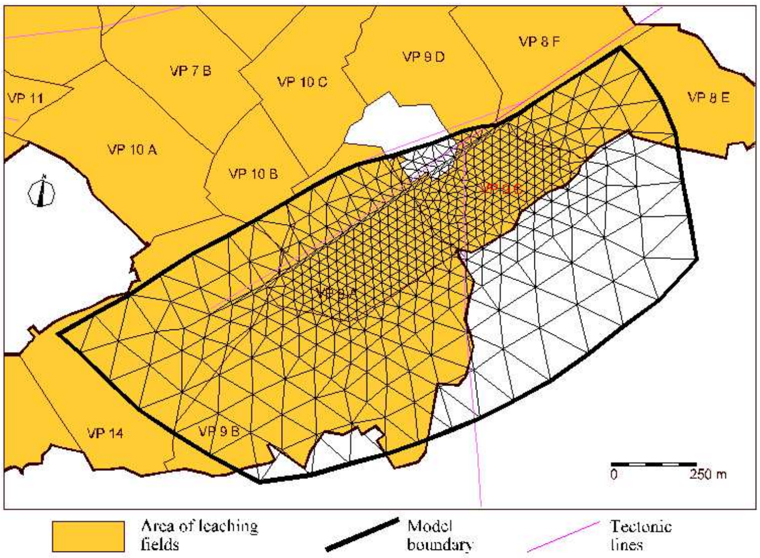


FIG. 2. *Location and shape of the model mesh of VP-9C site.*

3.2. Calibration of model and results. The model was calibrated using real data from monitoring for the period from March 2000 to September 2001. The calculation was performed as the series of 19 steady problems for constant boundary conditions and abstraction scenarios in each month. The transport of the contaminants was calculated using 3 days time step. Table 1 shows the total list of the wells where the remediation abstraction was performed. On the fig. 3 we can see the location of each abstraction well within the VP-9C site.

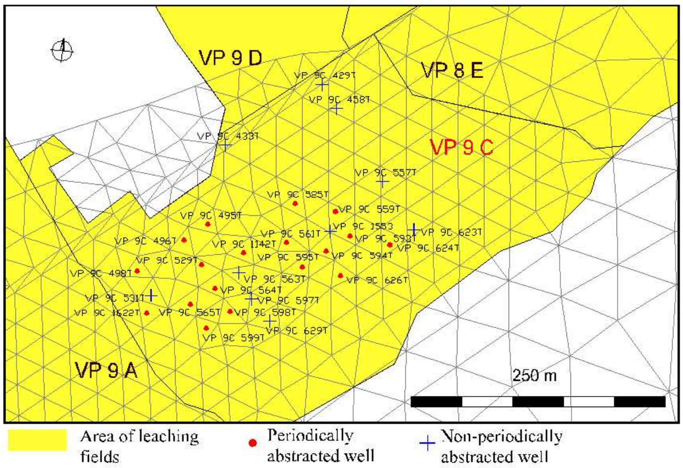
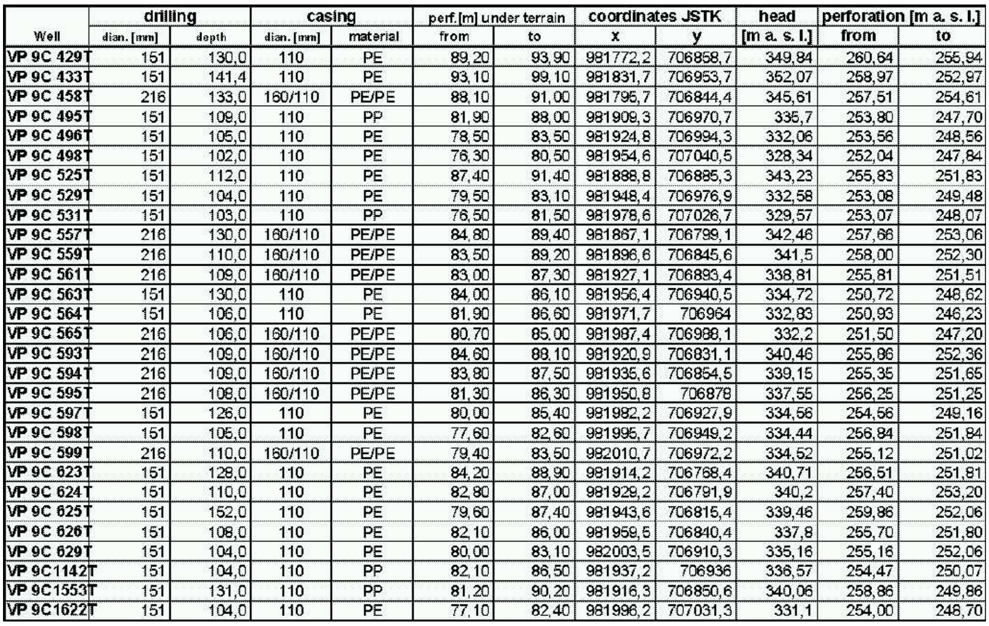


FIG. 3. *Location of abstraction wells within the VP-9C site.*



Well	drilling		casing		perf.[m] under terrain		coordinates JSTK		head	perforation [m a. s. l.]	
	dian. [mm]	depth	dian. [mm]	material	from	to	x	y	[m a. s. l.]	from	to
VP 9C 429T	151	130,0	110	PE	89,20	93,90	981772,2	706858,7	349,84	260,64	255,94
VP 9C 433T	151	141,4	110	PE	93,10	99,10	981831,7	706953,7	352,07	258,97	252,97
VP 9C 458T	216	133,0	160/110	PE/PE	88,10	91,00	981795,7	706844,4	345,61	257,51	254,61
VP 9C 495T	151	109,0	110	PP	81,90	88,00	981909,3	706970,7	335,7	253,80	247,70
VP 9C 496T	151	105,0	110	PE	78,50	83,50	981924,8	706994,3	332,06	253,56	248,56
VP 9C 498T	151	102,0	110	PE	76,30	80,50	981954,6	707040,5	328,34	252,04	247,84
VP 9C 525T	151	112,0	110	PE	87,40	91,40	981888,8	706885,3	343,23	255,83	251,83
VP 9C 529T	151	104,0	110	PE	79,50	83,10	981948,4	706976,9	332,58	253,08	249,48
VP 9C 531T	151	103,0	110	PP	76,50	81,50	981978,6	707026,7	329,57	253,07	248,07
VP 9C 557T	216	130,0	160/110	PE/PE	84,80	89,40	981867,1	706799,1	342,46	257,66	253,06
VP 9C 559T	216	110,0	160/110	PE/PE	83,50	89,20	981896,6	706845,6	341,5	258,00	252,30
VP 9C 561T	216	109,0	160/110	PE/PE	83,00	87,30	981927,1	706893,4	338,81	255,81	251,51
VP 9C 563T	151	130,0	110	PE	84,00	86,10	981956,4	706940,5	334,72	250,72	248,62
VP 9C 564T	151	106,0	110	PE	81,90	86,60	981971,7	706964	332,83	250,93	246,23
VP 9C 565T	216	106,0	160/110	PE/PE	80,70	85,00	981987,4	706988,1	332,2	251,50	247,20
VP 9C 593T	216	109,0	160/110	PE/PE	84,60	88,10	981920,9	706831,1	340,46	255,86	252,36
VP 9C 594T	216	109,0	160/110	PE/PE	83,80	87,50	981935,6	706854,5	339,15	255,35	251,65
VP 9C 595T	216	108,0	160/110	PE/PE	81,30	86,30	981950,8	706878	337,55	256,25	251,25
VP 9C 597T	151	126,0	110	PE	80,00	85,40	981982,2	706927,9	334,56	254,56	249,16
VP 9C 598T	151	105,0	110	PE	77,60	82,60	981995,7	706949,2	334,44	256,84	251,84
VP 9C 599T	216	110,0	160/110	PE/PE	79,40	83,50	982010,7	706972,2	334,52	255,12	251,02
VP 9C 623T	151	128,0	110	PE	84,20	88,90	981914,2	706768,4	340,71	256,51	251,81
VP 9C 624T	151	110,0	110	PE	82,80	87,00	981929,2	706791,9	340,2	257,40	253,20
VP 9C 625T	151	152,0	110	PE	79,60	87,40	981943,6	706815,4	339,46	259,86	252,06
VP 9C 626T	151	108,0	110	PE	82,10	86,00	981959,5	706840,4	337,8	255,70	251,80
VP 9C 629T	151	104,0	110	PE	80,00	83,10	982003,5	706910,3	335,16	255,16	252,06
VP 9C1142T	151	104,0	110	PP	82,10	86,50	981937,2	706936	336,57	254,47	250,07
VP 9C1553T	151	131,0	110	PP	81,20	90,20	981916,3	706850,6	340,06	258,86	249,86
VP 9C1622T	151	104,0	110	PE	77,10	82,40	981996,2	707031,3	331,1	254,00	248,70

Table 1
List of the remediation wells on VP-9C site.

The first phase of calibration was the setting and correction of initial conditions obtained by logging. Then the comparison of global balances in dependence on the active and total porosity and diffusion rate was performed. For each trial calculation the deviations (observed value minus calculated value) of mass in each month and their squares were computed. The sums of deviations and their squares for the whole calculation period are two target functions that we would like to minimize by changing of material parameters. The basic set of values of material parameters is shown in table 2.

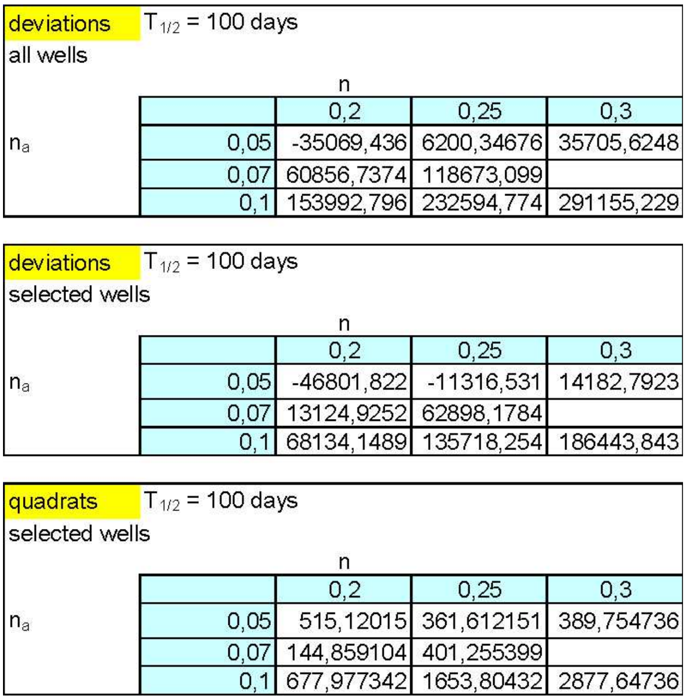
Active porosity n_a	0,05	0,07	0,1
Total porosity n	0,2	0,25	0,3
Diffusion rate $T_{1/2}$ **(days)**	50	100	150

Table 2
The basic set of values of material parameters.

The calibration of material parameters was performed in 3 steps. In each step always the one of the parameters is constant and the other two are varying. Table 3 shows the results for the step 1 where the $T_{1/2} = 100$ days.

After performing the all 3 steps we get intervals for values of material parameters, see table 4.

The time distribution of deviation of mass balance for values of $n = 0,27, n_a = 0,07$ and $T_{1/2} = 150$ days we can see on fig. 4. On the fig. 5 we can see the comparison of concentrations of SO_4^{2-} measured and calculated for limit values of parameters obtained by calibration process on the well VP 9C 565T.



deviations $T_{1/2}$ = 100 days
all wells

		n		
		0,2	0,25	0,3
n_a	0,05	-35069,436	6200,34676	35705,6248
	0,07	60856,7374	118673,099	
	0,1	153992,796	232594,774	291155,229

deviations $T_{1/2}$ = 100 days
selected wells

		n		
		0,2	0,25	0,3
n_a	0,05	-46801,822	-11316,531	14182,7923
	0,07	13124,9252	62898,1784	
	0,1	68134,1489	135718,254	186443,843

quadrats $T_{1/2}$ = 100 days
selected wells

		n		
		0,2	0,25	0,3
n_a	0,05	515,12015	361,612151	389,754736
	0,07	144,859104	401,255399	
	0,1	677,977342	1653,80432	2877,64736

TABLE 3
Deviations and squares for the step 1.

	min	max
Total porosity n	0,25	0,27
Active porosity n_a	0,07	0,08
Diffusion rate $T_{1/2}$ **(days)**	120	150

TABLE 4
Resulting intervals of material parameters.

REFERENCES

[1] Maryška, J.: *Existence, uniqueness and approximation of the hybrid-mixed formulation of the porous media flow problem,* Technical Report 635, ICS AS CR 1994.

[2] Maryška, J., Mužák, J.: *Hybrid-mixed model of the transport of the chemical substances,* In Proceedings of Numerical Modelling in Continuum Mechanics, Prague, Volume Part II (1994), 181 – 189.

[3] Maryška, J., Mužák, J.: *Mathematical modelling of the transport of chemical species in the contaminated underground water,* In Bourgeat, A. P., Carraso, C., Luckhaus, S. and Mikelič, A., editors, Proceedings of the Conference Mathematical Modelling of Flow Through Porous Media, St. Etienne, France, May 22 – 26, World Scientific (1995), 450 – 459,

[4] Maryška, J., Rozložník, M. and Tůma, M.: *Mixed-hybrid finite element approximation of the potential fluid problem,* J. Comput. Appl. Math. **63** (1995), 383 – 392.

[5] Maryška, J., Mužák, J. ND Hokr, M.: *Modelling of the Intercollector Transfer of the Contaminants,* Future Groundwater at Risk, Lisbon, 2001.

[6] Maryška J., Mužák J., Novák J. and Severýn: *Control of Remediation of Uranium Deposit Straz with Use of Numerical Modelling Approach,* Future Groundwater at Risk, Lisbon, 2001.

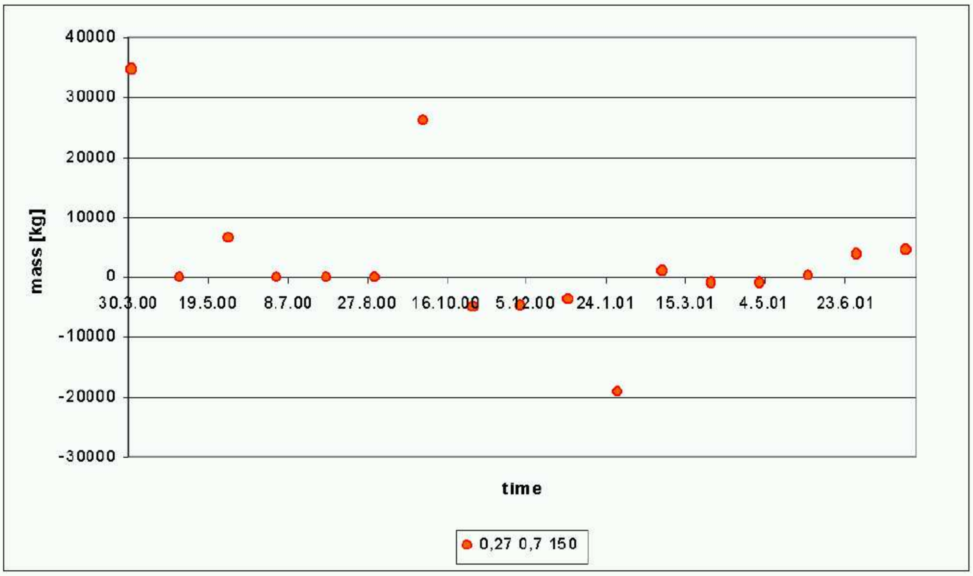


FIG. 4. *Time distribution of deviation of mass balance for values of* $n = 0,27, n_a = 0,07$ *and* $T_{1/2} = 150$ *days.*

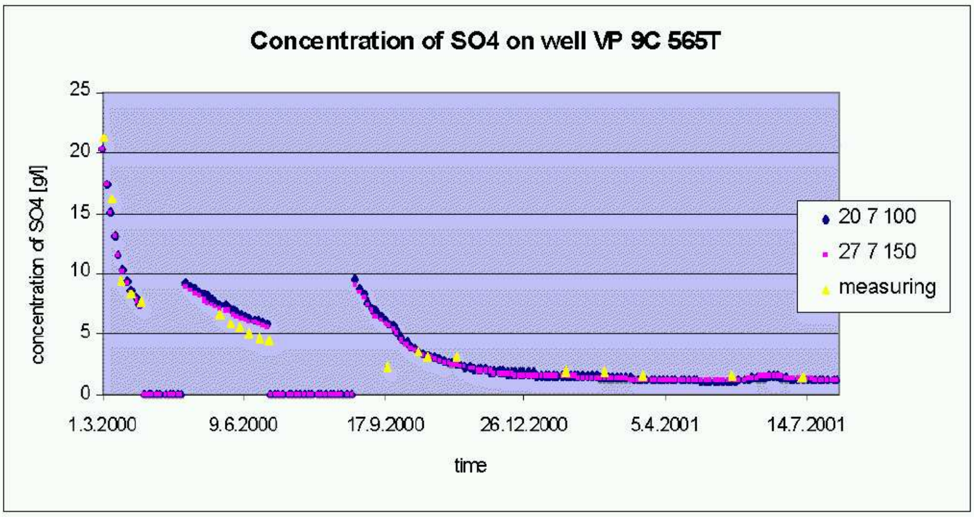


FIG. 5. *Comparison of concentrations of* SO_4^{2-} *measured and calculated (using two sets of values* $n = 0,20, n_a = 0,07, T_{1/2} = 100$ *days and* $n = 0,27, n_a = 0,07, T_{1/2} = 150$ *days) on well VP 9C 565T*

[7] Coats K. H., Smith B.D.: *Dead end pore volume and dispersion in porous media,* Soc. Pet. Eng. J. **4** (1964), 73–84.

[8] Gerke H.H., van Genuchten M. T.: *A dual-porosity model for simulating the preferential movement of water and solutes in structured porous media,* Water Resour. Res. **29** (1993), 305–319.