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APPLICATION OF A MODIFIED ANALYTICAL SOLUTION OF TRANSPORT EQUATION TO DETERMINE LONGITUDINAL DISPERSIVITY

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ABSTRACT

The column tests are suitable tools to determine the transport parameters of the investigated porous media. The measurement protocol is simple and the originated data can improve the accuracy of mass transport calculations. In our work we performed labor experiments to determine the dispersion coefficient of the waste dump material of Rudabánya. In these experiments a unit concentration of pollutant was injected into the column and the spread of this pollutant was observed in time. The Dirac-function describes the concentration change in the function of time and distance. By minor conversion the independent variable of this function (time) could be changed to volume. In this paper we would like to introduce the application of this modified function. We used curve fitting method on the data of experiments to determine the longitudinal dispersivity of waste dump material which was found 7 cm. In the following transport modeling work we could integrate the result of this experiment into the models and we could start to investigate the adsorption process of heavy metals in the waste dump matter.

INTRODUCTION

In Rudabánya several ores of zinc, copper, lead and cadmium were originated near iron ores by hydrothermal processes. During decades of mining activity a lot of waste dumps were created with high heavy metal content. In our previous research works the significant heavy metal content of these waste dumps have already been proven by sequential extraction investigations *(Tóth & Kovács, 2013)*. Not only the total heavy metal content but also the mobile element content is high in the waste dumps that means the elements can mobilize by effect of weak acids. In our present work column tests were performed to determine the transport parameters of the waste dumps material to prepare the contaminant transport simulations of mobile heavy metal compounds.

The column tests are applicable tools to calculate the dispersion coefficient *(Czinkota et al., 2006)*.

The basis of calculation is the one-dimensional form of transport equation *(Kovács, 2004, Kinzelbach, 1986)*:

$$\frac{\partial C}{\partial t} = \frac{\alpha_L \bar{v}_x}{R}\frac{\partial^2 C}{\partial x^2} - \frac{\bar{v}_x}{R}\frac{\partial C}{\partial x} - \lambda C \,. \tag{1}$$

In case of an instantaneous injection of pollutant mass M in the spatial point x = 0 and at time t = 0. This initial condition could be described by Dirac-function:

$$C_\delta(x,0) = \frac{\Delta M}{n_0 mwR}\delta(x)\,. \tag{2}$$

The Dirac-function $\delta(x)$ is defined by

$$\delta(x) = 0 \text{ for } x \neq 0\,,\ \int_{-\infty}^{\infty} \delta(x)dx = 1 \text{ for } x = 0\,. \tag{3}$$

Further demand that the solution is bounded, this means

$$C_\delta(\pm\infty, t) = 0\,. \tag{4}$$

In this case the solution of equation 1. that satisfied equation 2 and 4 is the Gauss-function.

$$C(x,t) = \frac{M}{2wmn_0 R\sqrt{\frac{\pi\alpha_L \bar{v}_x t}{R}}} \exp\left(-\frac{\left(x - \frac{\bar{v}_x t}{R} \right)^2}{\frac{4\alpha_L \bar{v}_x t}{R}} \right) \exp(-\lambda t) \tag{5}$$

where: *M* is the mass of pollutant, *w* is the infinitesimally small width of aquifer, m is the thickness of aquifer, n_0 is the porosity of aquifer, *R* is the reduction factor about the adsorption of pollutant, $\alpha_L$is the longitudinal dispersivity, $\bar{U}_x$ is the average velocity of seepage, *t* is the time, *x* is the distance and λ is the decay constant.

MATERIALS AND METHODS

In Equation 5. the concentration is the function of distance (x) and time (t). By a conversion we could change the second independent variable from time (t) to volume of effluent fluid (q).This change is based on the Darcy-function.

$$Q = K \cdot A \cdot I \tag{6}$$

where *K* is the hydraulic conductivity, *A* is the flow cross-section, *I* is the hydraulic gradient and *Q* is the discharge where $Q = \frac{q}{t}$.

The average velocity of seepage is determined by the following expression.

$$\bar{v}_x = K \cdot I \, . \tag{7}$$

To substitute Equation 7 into Equation 6 :

$$\bar{v}_x \cdot t = \frac{q}{A} \, . \tag{8}$$

This conversion is practical because the measuring of volume is comfortable and it could be more accurate than measuring of time.

After substitution of Equation 8 into Equation 5 the Gauss-function could be modified:

$$c(x,t) = \frac{M}{2wmn_0 R\sqrt{\dfrac{\pi\alpha_L \dfrac{q}{A}}{R}}} \exp\left(-\frac{\left(x - \dfrac{\left(\dfrac{q}{A}\right)}{R} \right)^2}{\dfrac{4\alpha_L \dfrac{q}{A}}{R}} \right) \exp(-\lambda \frac{q}{A\bar{v}_x}) \tag{9}$$

where *q* is the volume of effluent fluid.

Column test was performed to determine longitudinal dispersivity. This transport parameter could be determined in this indirect measurement by curve fitting method on measured data. The best fitting of function is found by iteration of non-measurable parameters.

Some parameters of function could be measured. A 53 cm high plastic column was filled up with waste dump sample. The cross-section of column was A = 10.17 cm^2. In time t = 0 a high concentration of manganese solution was injected in the system. The total mass of manganese was M = 274 mg. The flow of water inside the column was continuous before injection. The manganese solution was seeped thought the column with a constant velocity (v = 0.002 m/s). The effluent fluid was collected on the outflow side of column. The time and the volume of collected sample were registered, simultaneously. The outflow solution was collected in approximately 25 cm^3 units. The effective volume of each unit was determined after mass measuring and dividing by density of solution. After filling up of each unit the related time was registered.

RESULTS

First of all the original Gauss-function was fitted on measured data. The measured concentration was graphed in function of time (*Figure 1*). The correlation coefficient of fitted curve was r^2=0.91. The values of fitted parameters are presented in *Table 1*.

The fitting of modified Gauss-function is displayed in *Figure 2*. By application of this function a better fitting was experienced. The correlation coefficient of curve is r^2 = 0.93. The values of fitted parameters are presented in *Table 2*.

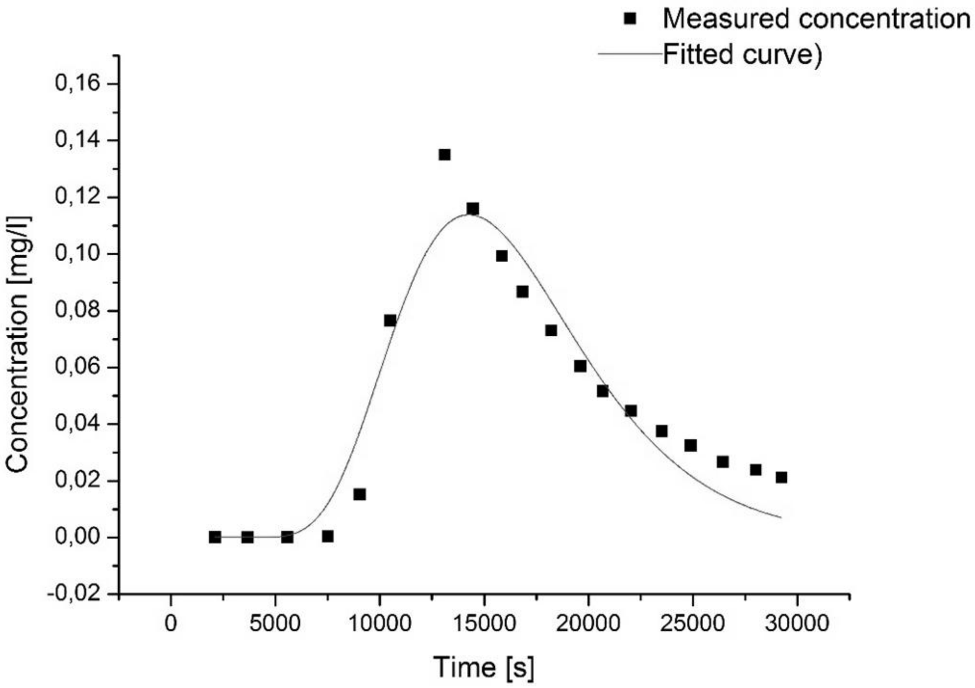

Figure 1. The measured concentration in function of time

Table 1

Values of fitted and measured parameters when the concentration is graphed in function of time

	Mass of pollutant M mg	**Cross-section** A cm^2	**Porosity** n_0 –	**Retardation factor** R –	**Longitudinal dispersivity** α_L cm	**Average velocity of seepage** v cm/s	**Distance** x cm	**Decay constant** λ 1/d
Value	274	10.17	0.35	0.80061	3.5521	0.002	52.7	0.0001737
Error	No fit	No fit	No fit	0.03769	0.60274	No fit	No fit	$8.538 \cdot 10^{-6}$

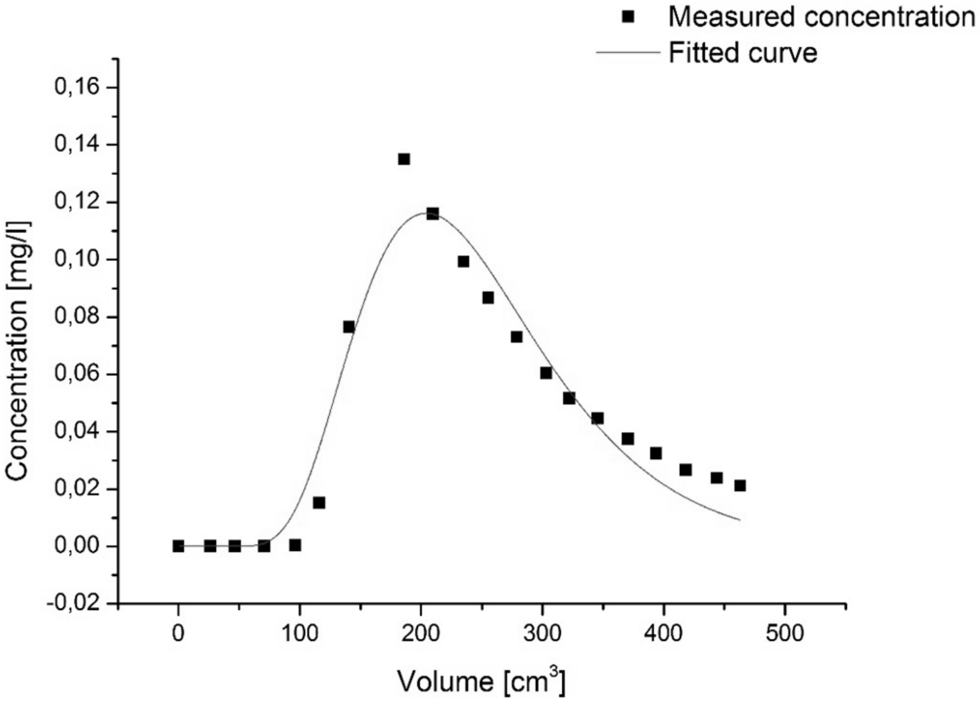

Figure 2. The measured concentration in function of volume of effluent fluid

Table 2

Values of fitted and measured parameters when the concentration is graphed in function of volume of effluent fluid

	Mass of pollutant	**Cross-section**	**Porosity**	**Retardation factor**	**Longitudinal dispersivity**	**Average velocity of seepage**	**Distance**	**Decay constant**
	M	A	n_0	R	α_L	v	x	λ
	mg	cm^2	–	–	cm	cm/s	cm	1/d
Value	274	10.17	0.35	0.69316	6.16084	0.002	52.7	$2.21 \cdot 10^{-4}$
Error	No fit	No fit	No fit	0.0423	1.01664	No fit	No fit	$1.22 \cdot 10^{-5}$

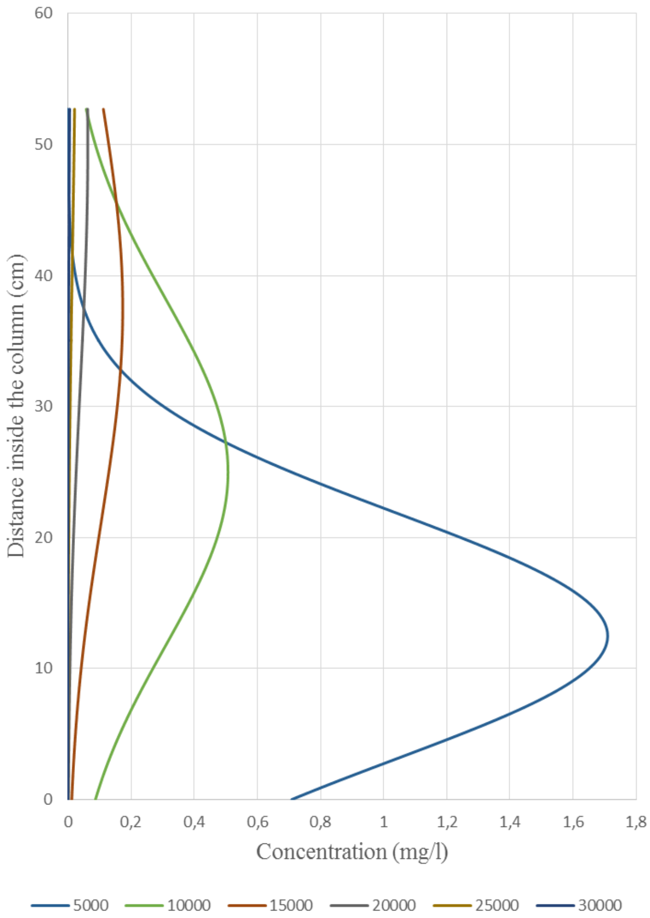

Figure 3. The concentration change of manganese solution along the column in different moments (unit of time: second)

CONCLUSIONS

In our previous works the longitudinal dispersivity of waste dump samples of Rudabánya have already been defined in breakthrough curve experiments *(Tóth et al., 2014)*. The breakthrough curve could be described by another one-dimensional solution of transport equation so the longitudinal dispersion could be determined with the same curve fitting method which method was introduced in this article. The calculated value of longitudinal dispersivity was 7 cm in the breakthrough curve experiment. In this investigation we could see the values of fitted parameters are largely depends on accuracy of measured parameters. In case of original function the correlation coefficient of best fitting is 0.91. The iterated parameter of longitudinal dispersivity is 3.5 cm.During application of modified Gauss-function the fitting of curve is better than in case of the original form of the function. Furthermore the determined value of longitudinal dispersivity is nearly 7 cm (6.16 cm) by fitting of the modified Gauss-function as like as in case of breakthrough curve experiment *(Tóth et al., 2014)*.

The concentration of effluent fluid could be graphed as a function of time or distance (Equation 9). After determination of fitted parameters of Gauss-function we could determine the concentration distribution of manganese solution along the column in different moments. In this case the concentration is the function of distance. (*Figure 3*) The graph shows the nonconservative case of pollutant distribution in different location and time because the value of decay constant $\lambda$is greater than 0 so the area under the curve is decreased more than the run out amount of pollution.

During measurement the decreasing of pollutant was observed because of irreversible adsorption of manganese. This process could be approximated by application of decay but it needs a better formula to describe the irreversible adsorption which process could be a kind of mineralization in case of waste dumps. In our following work we would like to investigate the irreversible adsorption and we would like to give a formula on it.

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