UDC 622.277

SUBSURFACE REACTIVE TRANSPORT PROCESSES MODELING

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The purpose of this article was analysis of such physical properties such as intrinsic permeability, dispersion, diffusion and advection. They are important input data to simulate reactive transport processes in subsurface. To obtain these parameters, we injected through the media a conservative non-reactive tracer (Br^-). The objective of this article was two-fold: to get us familiar with the solution to advection-dispersion equations; understand how different parameters (flow rate and dispersivity) affect the shape of breakthrough curves and spatial distribution of tracer's concentration at different times. For systems with constant dispersion and different flow rates was found that at low velocity dispersion is dominated by advection. Also, the dispersion predominance of advection at low flow rates was found for systems with constant flow rate and different values of dispersion.

Key words: permeability, solute, diffusion, advection, dispersion.

МОДЕЛЮВАННЯ ПІДЗЕМНИХ РЕАКТИВНИХ ТРАНСПОРТНИХ ПРОЦЕСІВ

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Проаналізовано такі фізичні властивості, як внутрішня проникність, дисперсність, дифузія та адвекція. Вони є важливими даними для моделювання підземних реактивних транспортних процесів. Для отримання цих параметрів застосований трасер (Br^-), який не вступає у реакції з оточуючим середовищем. Розв'язані рівняння адвекції та дисперсії, пояснено, як різні параметри (швидкість потоку та дисперсність) вливають на форму кривих і розподіл концентрації трасера у різні моменти часу. Представлені результати моделювання, що показують зміну в часі концентрації введеного в імітовану колону піску трасера (Br^-), при різних швидкостях потоку та дисперсностях. Переважання дисперсією адвекції, при низьких значеннях швидкостей потоків, було встановлено і для систем зі сталою швидкістю потоку та різними значеннями дисперсності.

Ключові слова: проникність, розчин, дифузія, адвекція, дисперсія.

PROBLEM STATEMENT. A solute in water will move from an area of greater concentration toward an area where it is less concentrated. This process is known as diffusion. Diffusion will occur as long as concentration gradient exist, even if the fluid is not moving. The mass of fluid diffusing is proportional to the concentration gradient, which can be expressed as Fick's first low: [1]

$$F = -D_d (dc/dx), \tag{1}$$

where F – mass flux of solute per unit area per unit time; D_d – diffusion coefficient (L^2/T); C – solute concentration (M/L^3); dC/dx – concentration gradient $(M/L^3/L)$.

The negative sign indicates that the movement is from areas of greater concentration to those of lesser concentration.

For systems where the concentrations are changing with time, Fick's second low applies.

Diffusion will cause a solute to spread away from the space where it is introduced into a porous medium, even in the absence of ground-water flow [2, 3]. Fig.1. shows the distribution of a solute introduced at concentration C_0, at time t_0, over an interval (x–a) to (x+a). At times t_1 and t_2, the solute has spread out, resulting in a lower concentration over the interval (x–a) to (x+a) but increasing concentrations outside of this interval.

Dissolved solids are carried along with the flowing ground water. This process is called advective transport. The amount of solute that is being transported is a function of its concentration in the ground water and the quantity of the ground water flowing [4].

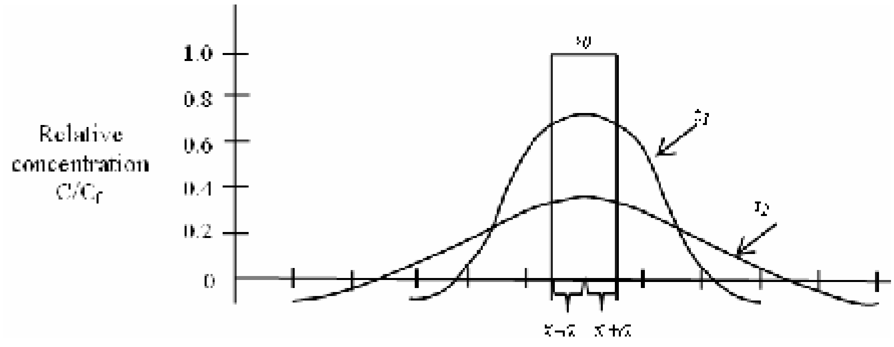

Figure 1 – Spreading of a solute slug with time due to diffusion [1]

The one-dimentional mass flux, *Fx*, due to advection is equal to the quantity of water flowing times the concentration of dissolved solids.

$$F_x = n_x \cdot n_e \cdot C, \tag{2}$$

where n_x - average linear velocity, n_e –effective porosity, C – solute concentration.

The one-dimensional advective transport equation is:

$$\frac{dC}{dt} = -n_x \frac{dC}{dx}. \tag{3}$$

Due to the heterogeneity of geologic materials, advective transport in different strata can result in solute fronts spreading at different rates in each stratum. Due to the fact that advection will transport solutes at different rates in each stratum, the composite sample may be a mixture of water containing the transported solute coming from one stratum and uncontaminated ground water coming from the different stratum, where the average linear velocity is lower. The concentration of the contaminant in the composite sample would thus be less than in the source [1].

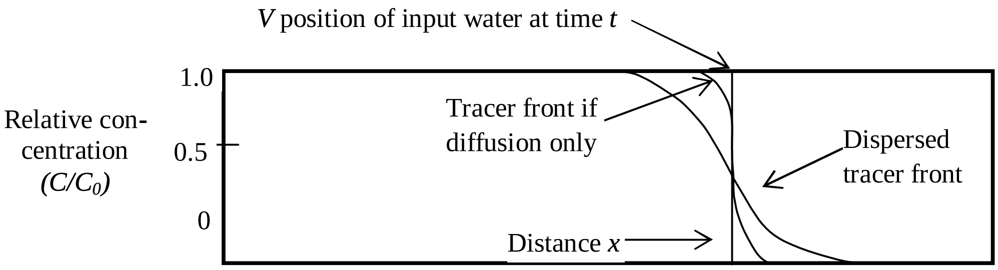

Figure 2 – Advective transport and the influence of longitudial dispersion and diffusion on the transport of a solute in one-dimensional flow [2]

The invading solute-containing water is not all travelling at the same velocity, mixing occurs along the flowpath. This mixing is called mechanical dispersion, and it results in a dilution of the solute at the advancing edge of flow fig.3. The mixing that occurs along the direction of the flowpath is called longitudial dispersion [1, 7].

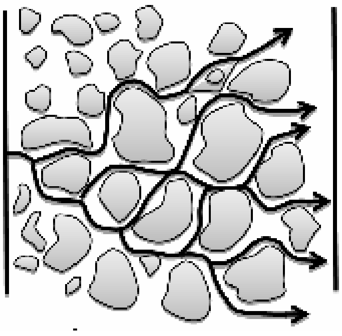

Figure 3 – Flowpaths in a porous medium that cause lateral hydrodynamic dispersion [2]

EXPERIMENTAL PART AND RESULTS OBTAINED. We were doing a sand column experiment Fig.4. The column was 30 cm long, with a porosity of 25%. A Tracer (Br-) was injected into the column. This column was simulated by dividing it into 100 elements, each 0.3 m long.

We run our simulation under the following conditions: 1) a Darcy flow velocity of 1.0 cm/day, 5.0 cm/day, and 25.0 cm/day, with fixed dispersivity of 2.0 cm., 2) with a constant Darcy flow velocity of 25.0 cm /day, and a dispersivity value of 0.01 cm, 2.0 cm, and 50.0 cm.

This gave us 6 different simulations. For the output of simulations we wanted to do the following:

1) for the simulation with flow velocity of 5.0 cm/day and dispersivity of 2.0 cm, to draw the concentration spatial profiles of the tracer at different times and explain why the shape of the curves are different at different times;

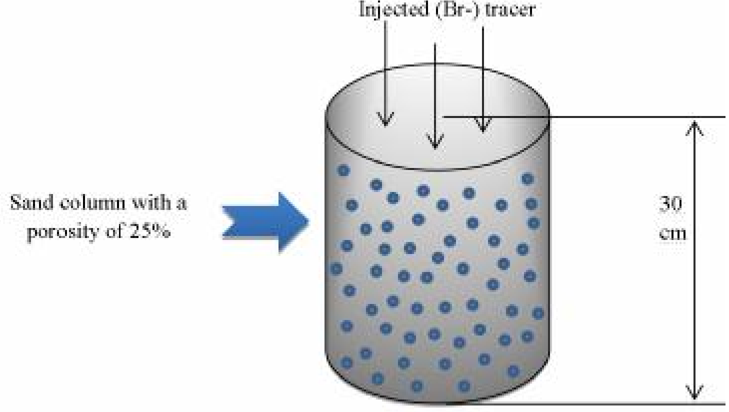

Figure 4 – Sand column experiment with the injected tracer

2) draw figures to compare the breakthrough curves with the same dispersivity (2.0 cm) but different flow velocities (1.0 cm/day, 5.0 cm/day, and 25.0 cm/day). Explain what causes the differences in the shape of the curves;

3) draw figures to compare the breakthrough curves with the same velocity (25.0 cm/day) but different dispersivity values (0.01 cm, 2.0 cm, and 50.0 cm). Explain what causes the differences in the shape of the curves.

Modeling was done by using CrunchFlow (software for modeling multicomponent reactive flow and transport). We successfully run all our input files under stated above conditions Fig. 5.

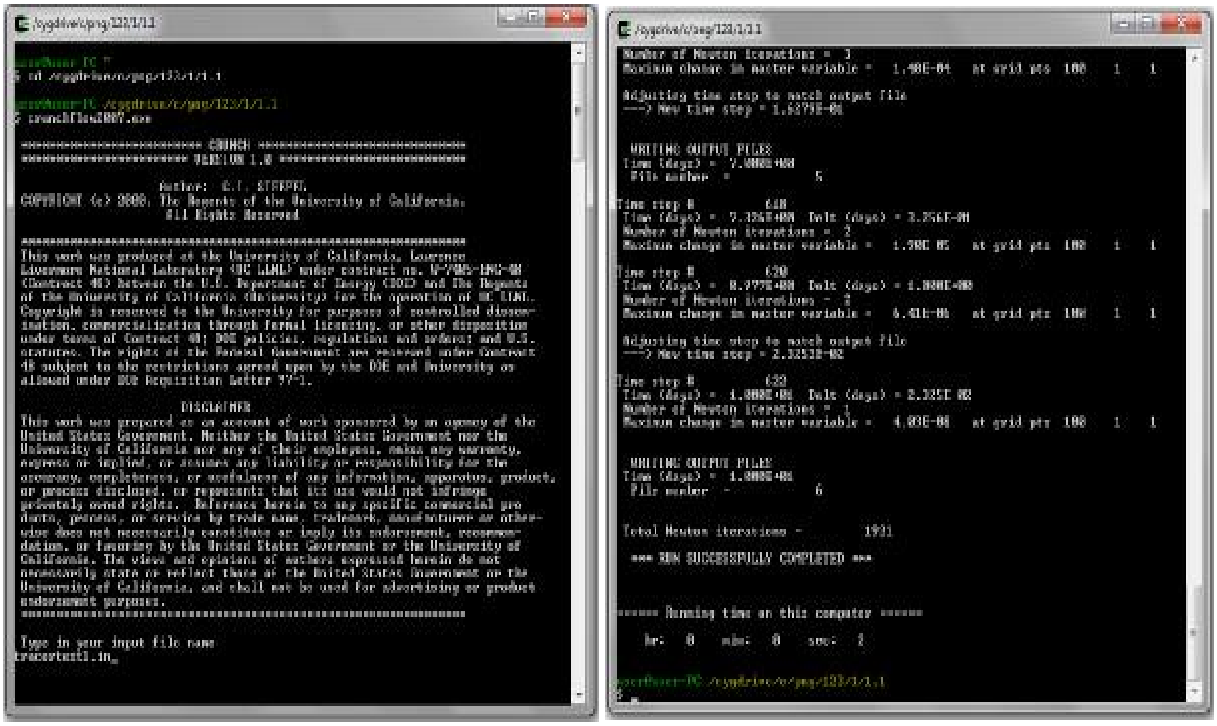

Figure 5 – Modeling environment of CrunchFlow software

We used Excel software to draw the curves from all our output files Fig.6-8. All of them are presented below.

Initially (0.001 day), when the tracer is introduced into the inlet of the porous system, its spatial profile is step-like. At this moment the solute has yet to have enough time to disperse.

As time progresses (from 1 to 2 days), the solute is transported by two mechanisms, advection and dispersion/diffusion. If only advection were at work the spatial profile of the tracer concentration would progress across the porous system with a step-like profile, but due to the dispersion (rate of diffusion is considered to be negligibly small in comparison to rate of dispersion) of the solute, the concentration of the solute becomes spatially-heterogeneous. Dispersion results in solute particles traversing the porous medium at different rates, and thus creating a “smeared out” concentration profile.

Beyond the fourth day, the advection of the solute experiencing the greatest amount of retardation by the effect of dispersion that has traversed the entire porous system; thereby the system is now homogenously with the tracer.

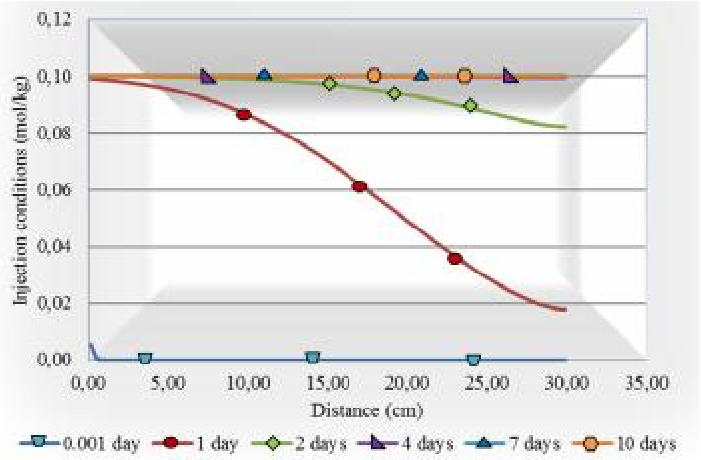

Figure 6 – Concentration spatial profiles of tracer with flow velocity of 5.0 cm/day and dispersivity of 2.0 cm at different times

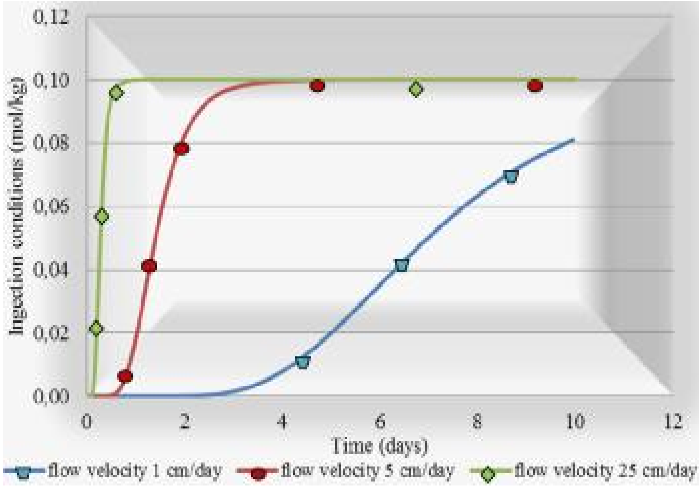

Figure 7 – Breakthrough curves for a system with dispersivity of 2.0 cm and ungoing variable flow rates

The differences that we are observed in the curves are related to two methods of fluid conveyance, advection and dispersion. When the ratio of the advection to dispersion is high (flow velocity=25 cm/day) the breakthrough curves will appear more step-like, as concentration of tracer has not been smeared out by dispersion. When the ratio of advection to dispersion is low (flow velocity 1 cm/day) the breakthrough curve is smeared out by the previously mentioned effects of dispersion. The range of flow velocities on the spatial range considered shows very different breakthrough curves, with ratios of advection to dispersion of 12.5, 5.

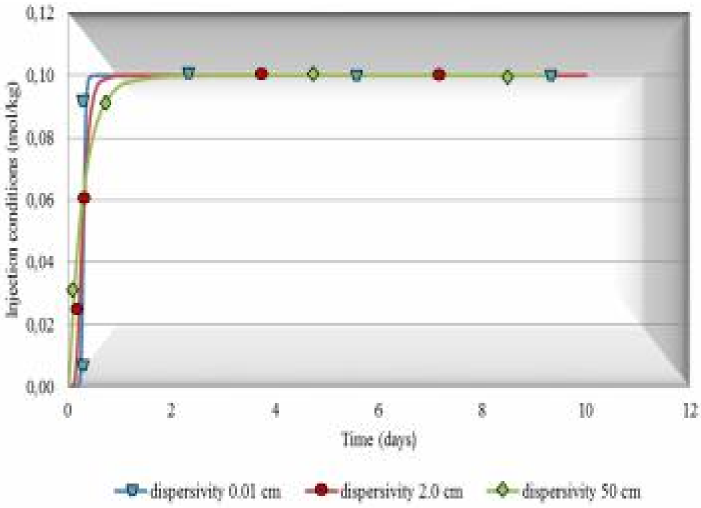

Figure 8 – Breakthrough curves for a system with flow velocity 25.0 cm/day and undergoing variable dispersivities

The differences that are observed in the curves are related to two methods of fluid conveyance, advection and dispersion. When the ratio of the advection to dispersion is high (dispersivity 0.01 cm) the breakthrough curves will appear more step-like, as the concentration of tracer has not been smeared out by dispersion.

When the ratio of advection to dispersion is low (dispersivity 50.0 cm) the breakthrough curve is smeared out by the previously mentioned effects of dispersion.

The range of dispersivities on the spatial range considered shows very similar breakthrough curves, unlike when considering the different flow velocities, with ratios of advection to dispersion of 2500, 12.5, and 0.5.

These ratios are larger than those, when previously flow velocities were varied, yet the breakthrough curves are quite similar, this demonstrates the dominance of advection over dispersion in our system.

CONCLUSIONS. For conditions with flow velocity of 5.0 cm/day and dispersivity of 2.0 cm at different times we observed that beyond the fourth day, the advection of the solute experiencing the greates amount of retardation by the efects of dispersion; after that period of time the system was homogenously saturated with the tracer.

For a system with dispersivity of 2.0 cm and different flow velocities we observed that dispersion dominated advection at low flow velocities.

For a system with flow velocity 25.0 cm/day and different dispersivity values we observed that dispersion again dominated advection at low flow velocities.

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МОДЕЛИРОВАНИЄ ПОДЗЕМНЫХ РЕАКТИВНЫХ ТРАНСПОРТНЫХ ПРОЦЕССОВ

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Проанализировані такие физические процессы, как внутренняя проницаемость, дисперсность, диффузия и адвекция. Они являются важными данными для моделирования подземных реактивных транспортных процессов. Для получения этих параметров применен трассер (Br^-), который не вступает в реакции с окружающей средой. Решены уравнения адвекции и дисперсии. Разъяснено, как разные параметры (скорость потока и дисперсность) воздействуют на форму кривых и распределение концентрации трассера в разные моменты времени. Представлены результаты моделирования, показывающие изменение во времени концентрации введенного в имитированную колону песка трассера (Br^-) при разных скоростях потока и дисперсностях. Превалирование дисперсии над адвекцией при низких значениях скоростей потоков установлено и для систем с постоянной скоростью потока и разных значениях дисперсности.

Ключевые слова: проницаемость, раствор, диффузия, адвекция, дисперсия.

Стаття надійшла 12.10.2012
Рекомендовано до друку
к.х.н., доц. Козловською Т.Ф.