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MODEL OF HYDROCARBONS TRANSPORT THROUGH THE POROUS GROUND MEDIA

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Dispersion model of hydrocarbons transport in porous media has been presented. Mathematical description of this process allows to estimate whether the menace of ground waters can occur as a result of hydrocarbons transport through the soil. The convection term in the mass transport equation is taken into account due to the higher velocity of propagation in vertical direction. Additionally, introduction to the balance equation the biosorption link allows to take into account microorganisms influence on impurities concentration, especially on heavy oils derived compounds. To verify the theoretical model series of the experiment in the soil filter has been carried out.

Keywords: petroleum derived products transport, hydrocarbons transport in soil, transport in porous media, the soil filter method.

Наведено модель дисперсії транспортування вуглеводнів у пористих середовищах. Математичний опис цього процесу дозволяє оцінити, чи є загроза ґрунтовим водам під час транспортування вуглеводнів через ґрунт. Термін конвекції в рівнянні перенесення маси враховується за рахунок вищої швидкості поширення у вертикальному напрямку. Крім того, введення в рівняння балансу посилання біосорбції дає змогу оцінити вплив кількості мікроорганізмів від концентрації домішок, особливо важких масел, отриманих сполук. Проведено серію експериментів з метою перевірки теоретичної моделі в фільтрі ґрунту.

Ключові слова: нафтопродукти транспорту, транспорт вуглеводнів в ґрунті, транспорт в пористих середовищах, метод фільтра ґрунту.

Introduction

Industry development stimulates the growth of request for products derived from rock oil. Unfortunately, many different kinds of harmful substances of varied constitution are included in these products, so they are the source of threat to the environment, especially because they may be transported from the surface of the ground to the surface of the underground waters [1]. Rock oil derived substances introduced into the ground are initially driven in perpendicular direction by dispersion forces through the ground aeration zone in which some amount of rock oil products is absorbed while other filters through the ground and often even reach the groundwaters mirror [2].

Transport of organic substances in the ground was analysed by several authors [3–8] but the problem of the mathematical description of this phenomenon is still opened. So the purpose of this paper is to present the method of analytic solution of the equation describing transport of organic substances being reduced to one direction.

1. Mathematical description of the hydrocarbons transport through the ground matrix

Let us consider the parabolic partial differential equation of the form

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial z^2} - \frac{\partial (vu)}{\partial z}. \qquad (1)$$

In order to solve the above equation we may use the well known method of solving the similar problem existing in the field of unsteady heat exchange. It is known that solution of the equation

$$\frac{\partial u}{\partial t} = \frac{1}{2}\frac{\partial^2 u}{\partial z^2} \qquad (2)$$

has the following form:

$$u(z,t) = \frac{1}{\sqrt{2\pi t}}\exp\left(\frac{-z^2}{2t}\right). \qquad (3)$$

Let introduce an auxiliary function of the form:

$$\tilde{u}(z,t) = u(z, \alpha \cdot t). \qquad (4)$$

It is easy to calculate that:

$$\frac{\partial \tilde{u}}{\partial t} = \alpha \frac{\partial u(z,\alpha t)}{\partial t}, \quad \frac{\partial^2 \tilde{u}}{\partial z^2} = \frac{\partial^2 u}{\partial z^2}. \qquad (5)$$

Combining the Eqs. (2) and (5) we may get the formula:

$$\frac{\partial \tilde{u}}{\partial t} = \frac{1}{2}\alpha \frac{\partial^2 \tilde{u}}{\partial z^2} \qquad (6)$$

from which it is easy to show that the function:

$$\tilde{u}(z,t) = u(z, 2Dt) \qquad (7)$$

performs the equation:

$$\frac{\partial \tilde{u}}{\partial t} = D\frac{\partial^2 \tilde{u}}{\partial z^2} \tag{8}$$

which solution may be presented in the following form:

$$\tilde{u}(z,t) = \frac{1}{\sqrt{4\pi Dt}}\exp\left(\frac{-z^2}{4Dt}\right). \tag{9}$$

Let us check what the equation is additionally fulfilled by the another auxiliary function of the form:

$$\hat{u}(z,\,t) = \tilde{u}(z - vt,\,t). \tag{10}$$

In a such case after combining eqs. (8) and (10) we obtain the following equation:

$$\frac{\partial \hat{u}}{\partial t} = \frac{\partial \tilde{u}}{\partial t} - v\frac{\partial \tilde{u}}{\partial z}; \tag{11}$$

$$\frac{\partial \hat{u}}{\partial t} = D\frac{\partial^2 \tilde{u}}{\partial z^2} - v\frac{\partial \tilde{u}}{\partial z} \tag{12}$$

and finally:

$$\frac{\partial \hat{u}}{\partial t} = D\frac{\partial^2 \hat{u}}{\partial z^2} - v\frac{\partial \hat{u}}{\partial z}. \tag{13}$$

So, the function $\hat{u}$ described by the equation of the following form:

$$\hat{u} = u(z - vt,\,2Dt) = = \frac{1}{\sqrt{4\pi Dt}}\exp\left(\frac{-(z - vt)^2}{4Dt}\right) \tag{14}$$

is the searching solution of eqn. (1),f or v = const.

2. Mathematical description of the hydrocarbons transport through the ground matrix with taking into account their mass decrement caused by the biochemical reaction

Let us consider the equation of the form:

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial z^2} - \frac{\partial (vu)}{\partial z} - \alpha\,z. \tag{15}$$

Searching for the solution of the above equation, being the developed form of eqn. (1), we may consider the following function:

$$\bar{u}(z,\,t) = \hat{u}\cdot\exp(-\alpha t). \tag{16}$$

The derivative of this function in respect of t is described as follows:

$$\frac{\partial \bar{u}}{\partial t} = -\alpha\hat{u}\exp(-\alpha t) + \frac{\partial \hat{u}}{\partial t}\exp(-\alpha t). \tag{17}$$

The above equations may be presented in the forms:

$$\frac{\partial \bar{u}}{\partial t} = -\alpha\bar{u} + \left(D\frac{\partial^2 \hat{u}}{\partial z^2} - v\frac{\partial \hat{u}}{\partial z}\right)\exp(-\alpha t) \tag{18}$$

or

$$\frac{\partial \bar{u}}{\partial t} = D\frac{\partial^2 \bar{u}}{\partial z^2} - v\frac{\partial \bar{u}}{\partial z} - \alpha\bar{u}. \tag{19}$$

So, the function $\bar{u}(z,\,t)$ described by eqn. (16) is the searching solution of eqn. (15) which may be presented in one of the following forms:

$$\bar{u}(z,\,t) = \exp(-\alpha t)\cdot\frac{1}{\sqrt{4\pi Dt}}\exp\left[-\frac{(z - vt)^2}{4Dt}\right] \tag{20}$$

or

$$\bar{u}(z,\,t) = \frac{1}{\sqrt{4\pi Dt}}\exp\left[-\frac{(z - vt)^2}{4Dt} - \alpha\,t\right]. \tag{21}$$

The function $\bar{u}(z,\,t)$ fulfils the following dependence

$$\int_{-\infty}^{+\infty}\bar{u}(z,\,t)\,dz = \exp(-\alpha t). \tag{22}$$

It is possible for practical applications, assuming the constant value of the diffusion coefficients D_i = const, to present the solution of the partial differential equation

$$\frac{\partial C_i}{\partial t} = D_i\frac{\partial^2 C_i}{\partial z^2} - \frac{\partial v C_i}{\partial z} - \mu_i C_i \tag{23}$$

in the following form:

$$C_i(z,t) = \frac{C_{io}S}{\sqrt{4\pi D_i t}}\exp\left\{-\left[\frac{(z - vt)}{4D_i t} + \mu_i t\right]\right\}. \tag{24}$$

Parameters of the above equation may be determined using the regression model [9].

3. Description of the soil filter method

In order to verify results obtained from theoretical models the soil filter with dry matrix were constructed. This column-shaped filter with the inside diameter of 135 mm and the height of 2000 mm was made of polypropylene and is a segmented structure consisting of 18 cylindrical test cells, each of the height of 100 mm and the outside diameter of 137 mm. The gravel layer, of the height of 200 mm, located at the bottom of the soil filter holds up all the cylindrical test cells. The scheme of this filter is shown in Fig. 1. The sand deposit was used as a model to simulate the penetration of petroleum contaminants from the soil surface towards underground waters.

The function of hydrocarbon concentration $C_i(z,\ t)$ described by eqn. (24), may be determined by measuring of the hydrocarbon concentration in each of the 18 segments of the column soil filter in relation to the assumed migration time.

Distribution of the selected hydrocarbon concentrations in the soil filter was experimentally determined after 24, 48, 96, 192 and 384 hours (it means after 1, 2, 4, 8 and 16 days). For example, distribution of isooctane and *n*-hexadecane concentrations obtained using the soil filter method is respectively shown in Fig. 2 and 3.

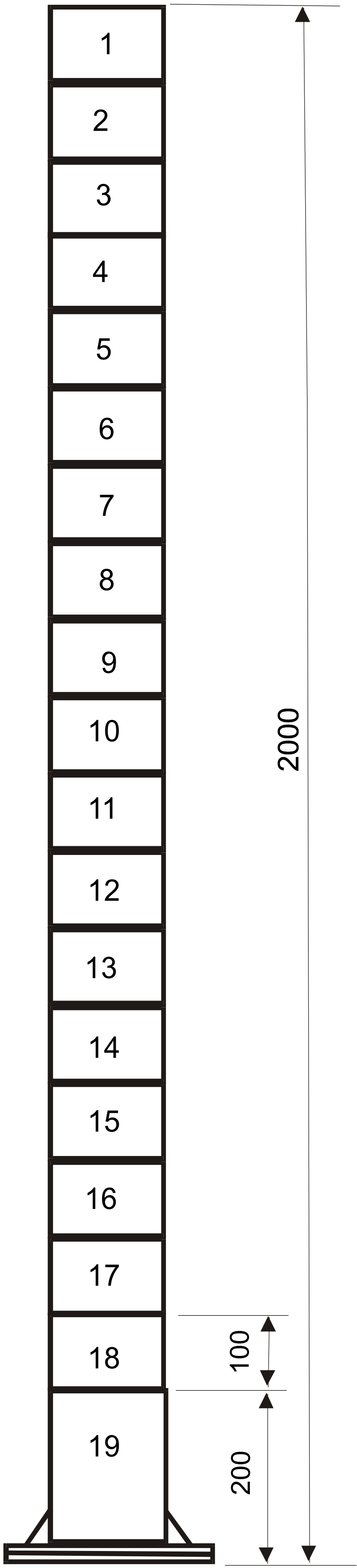

Fig. 1. Illustration of the soil filter method

Comparison of the results calculated from eqn. (24) with those obtained from the soil filter method will make possible not only to determine unknown diffusion coefficients D_i but also to choose the most useful for calculation transport model as well.

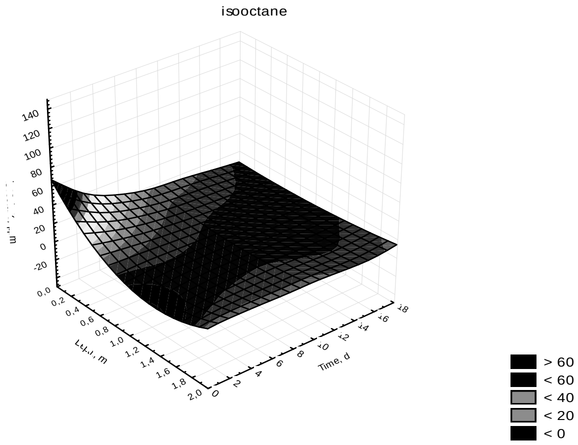

Fig. 2. Distribution of isooctane concentrations obtained in the soil filter

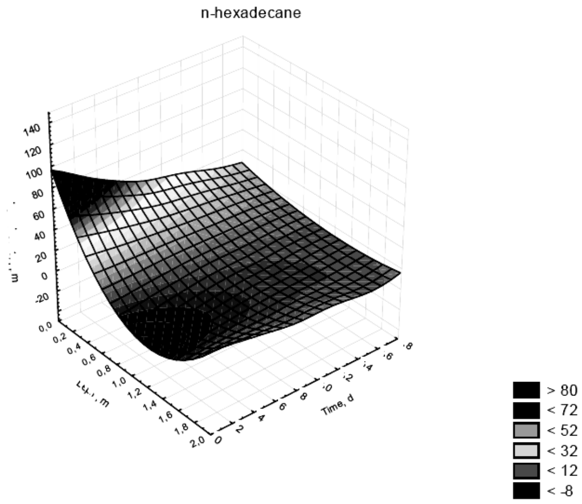

Fig. 3. Distribution of n-hexadecane concentrations obtained in the soil filter

Conclusions

The function $C_i(z, t)$, described by eqn. (24), being the solution of the mass balance equation (23), has to be determined in order to estimate the real threat of hydrocarbons being migrated through the ground especially in the perpendicular direction. Due to this function the time of hydrocarbons migration from the surface of the ground to the surface of the underground waters may be evaluated. Taking into account the convection term in eqn. (23) explains increase in velocity of hydrocarbons migration into orthogonal direction to the free surface of effluents.

Moreover, the last term of the right-hand side of eqn. (23) allows to consider the effect of microorganisms upon changes of hydrocarbons concentration in the soil. As hydrocarbons concentration in the system where their migration takes place is usually higher from that of bigenic elements (N, P) it may be assumed that the decomposition reactions of migrating hydrocarbons are of the first order [10].

The discrete function $C_i(z, t)$ may be experimentally determined by measuring the values of hydrocarbons concentrations in the soil filter in relation to the assumed migration time.

Notation

μ_i	–	hydrocarbons' biodegradation coefficient, $[s^{-1}]$
C_i	–	concentration of key component "*i*" in the matrix $[kg \cdot m^{-3}]$
C_{io}	–	initial concentration of key component "*i*" in the matrix, $[kg \cdot m^{-3}]$
D_i	–	equivalent diffusion coefficient of key component "*i*" $[m^2 \cdot s^{-1}]$
i	–	a symbol standing for the first letter of the tested hydrocarbon ($i = b, t, x, h, o$)
S	–	the maximum depth of hydrocarbon penetration through the ground, [m]
t	–	migration time, [s]
z	–	direction of hydrocarbons' migration, [m]

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