CONDITIONS FOR PHYSICAL MODELLING OF THE SPREAD OF CONTAMINANTS IN GROUNDWATER

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Abstract

The paper contains a review of dimensionless experimental dependencies determining the coefficient of transverse dispersion D_y. In the course of the dimensional analysis, dimensionless experimental dependencies describing the dispersion of pollutants in groundwater with hydraulic and physical parameters of soil in the case of steady and uniform groundwater motion were presented. The analysis allowed the determination of dimensionless practical relationships defining the dispersion factor in the perpendicular direction to the main flow direction.

Keywords: contaminants, groundwater, dispersion coefficient

1. INTRODUCTION

On the basis of the dimensional analysis, dimensionless experimental dependences between the dispersion coefficient values D_y and the hydraulic and physical parameters of the soil: k, I, d_{10} in the case of spreading pollutants by steady and uniform groundwater motion are shown.
Definition:
D_0 - the coefficient of molecular diffusion [m^2/s],

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D_y - the coefficient of dispersion in the direction perpendicular to the main flow direction [m^2/s],
d_{50} - the substitute diameter of the ground material [m],
d_{10} - the effective diameter of the ground material [m],
I - the groundwater table gradient [-],
k - the soil filtration coefficient [m/s],
v - the filtration velocity of groundwater [m/s],
υ - the coefficient of kinematic viscosity of water [m^2/s],
Pr - the Prandtl number [-],
Pe - the dynamic Péclet number [-],
Pe_m - the molekular Péclet number [-],
Re – the Reynolds number [-].

2. A LITERATURE ANALYSIS FOR DIMENSIONLESS EXPERIMENTAL DEPENDENCIES OF DISPERSION COEFFICIENT DY

It is widely accepted for determining the value of dispersion factor used the Prandtl number and Reynolds number in the form of general relationship:

$$Pr = a_1 Re^{b_1} \tag{1}$$

The above relationship was widely verified in the range of laminar water movement (Re $\leq$ 5) for soils whose substitute diameter $d_{50} \geq 1$ mm. As a result, experimental values of coefficients were obtained: $a_1 \in$ <0,11;1,70>, $b_1 \in$ <0,70;1,10>.
The research showed relatively large quantitative discrepancies between the coefficients a_1 and b_1, which was caused by various conditions in which the studies were performed [2].
When the scope of experimental studies was expended beyond the range of laminar motion ($5 \leq Re \leq 380$), the researchers found an increase in coefficients. For such groundwater flow conditions, the values of coefficients a_1 and b_1 increased respectively to 1.95 and 1.33, which was explained by the increase in resistance to motion at the turbulent flow of groundwater in the porous medium. Using the Prandtl number and the Reynolds number, the size of the dispersion coefficients was determined by referring the values of the Reynolds number to the value of the specific filtration coefficient k 'in the form:

$$Re^* = \frac{v\sqrt{k'}}{\upsilon} \tag{2}$$

where the specific coefficient k':

(3)

Based on the above relationships, it can be concluded that the dependence of $Pr = f(Re*)$ can only be used in the filtration of liquids with essentially different physical properties of the contaminant solution.

Other researchers [5] have made the D_y dispersion factor dependent on the following dimensionless products:

- the dynamic Péclet number $Pe = \frac{v\, d_{50}}{D_y}$,

- the molekular Péclet number $Pe_m = \frac{v\, d_{50}}{D_0}$,

- the Prandtl number,
- the Reynolds number .

In their research, among others A. E. Scheidegger [8] and P. G. Saffman [7] used the dynamic Péclet number and the molecular Péclet number in the form of the relationship $Pe = f(Pe_m)$ to determine the dispersion coefficient in the direction perpendicular to the main flow direction. The performed studies concerned the filtration velocity $v \leq 10^{-6}$ and the values of Reynolds numbers $Re \leq 10^{-4}$. Analyzing these studies, it can be concluded that the D_y dispersion factor related to the Péclet number can be determined only in cases involving low filtration velocities. Under such flow conditions, molecular diffusion plays a significant role in the phenomenon of the spread of contaminants and the molecular diffusion coefficient D_0 cannot be neglected.

Some authors used the dependence of the dynamic Péclet number and the Reynolds number in the form of the expression $Pe = f(Re)$ to determine the coefficient of transverse dispersion. Experimental studies verifying this dependence were mainly conducted in the field of turbulent flow. Their summary was conducted by W. E. Ranz [6] and T. Baron [3], who found that for turbulent flow the value of dynamic Péclet number $Pe \leq 11$, while for laminar flow ($Re \leq 5$), excluding inertial forces and resistance losses, the Péclet number may be smaller than its value in turbulent flow. Also other studies [1], [4] and our applied research confirmed this conclusion and showed that in the laminar flow range ($Re \leq 1$) the value of the Péclet number $Pe \leq 4$.

Other approach is presented by authors [9] examining the value of the coefficient of transverse dispersion, taking into account dependance $Pe = f(Re)$ including the stratified flow caused by the high concentration of flowing contaminant. In the course of own research it was found that rate of contaminants concentration do not affect the difference in pollutants and groundwater solution.

Summarizing experimental studies which determine value of D_y factor based on the Péclet number and Reynolds number it can be stated that research were conducted mainly with large-grained or stony ground with a wide range of filtration velocity ($10^{-7} \leq v \leq 10^{-1}$ m/s). For both dependencies the Reynolds number value was referred to the substitute diameter of ground d_{50} and in laboratory tests grounds with wide range of granulation ($0,20 \geq d_{50} \geq 40,00$ mm) were used. The dispersion coefficients were expressed in the form of dimensionless experimental dependencies taking into account:
- The Prandtl number and the Reynolds number,
- The Péclet number and the Reynolds number,
- The Péclet number and the molecular Péclet number.

The values of dispersion factors were related to the filtration velocity and the substitute diameter of the ground material d_{50}.

3. DIMENSIONLESS DEPENDENCIES SELECTION FOR DETERMINING D_Y COEFFICIENT

Observations mentioned during the literature analysis justify the usefulness of performing laboratory test to determine the coefficient of transverse disperssion based on dimensionless relationships in a relatively little researched range of ground granulation diameters ($0,50 \geq d_{50} \geq 1,00$ mm). The D_y factors were defined based on dimensionless relations taking into account:
- Prandtl number and Reynolds number in form Pr = f(Re) for grounds with diameter $d_{50} \leq 1$ mm instead of $d_{50} \geq 1$ mm,
- Péclet number and Reynolds number in form Pe = f(Re) for laminar flow (Re ≤ 5) instead of turbulent flow.

In both types of dimensionless dependencies values of Reynolds number were referred to the size of the effective diameter d_{10} instead of the substitute diameter d_{50} and the filtration coefficient k and the groundwater table gradient I instead of the filtration velocity v. The justification of using the k, I, d_{10} dependencies was presented in detail in the previous paper [2].
In the researches the indicator with the same viscosity and density as groundwater was used, that is why the Pr = f(Re*) dependence could not be applied in reference to k' factor. Moreover, because of considering the spread of contaminants in a stream of groundwater for Reynolds numbers Re $\geq 10^{-3}$ the value of molecular diffusion D_0 and relation Pe = f(Pe$_m$) were omitted in researches.

4. ANALYSIS OF THE SPREAD OF CONTAMINANTS IN GROUNDWATER AND SELECTION OF COEFFICIENTS WHICH DESCRIBE THEM

Analyzing the spread of contaminants in groundwater, seven parameters describing this phenomenon were identified:
- density of groundwater ρ_w,
- filtration coefficient k,
- difference in the height of water table Δh between the initial and final cross-section of the groundwater stream,
- the effective diameter of soil d_{10},
- length of the soil area L,
- the coefficient of kinematic viscosity of groundwater υ,
- the coefficient of contaminants dispersion D_y.

In further considerations the fictitious forces, centrifugal forces and, additionally, the phenomenon of capillary infiltration occurring in the ground due to negligible effect of the phenomenon on the time of infiltration of pollutants were omitted, also by other researchers.

5. DIMENSIONAL ANALYSIS

The following function of spreading pollutants in groundwater has been assumed:

$$f_1(D_y, k, \Delta h, L, d_{10}, \upsilon, \rho_w) = 0 \qquad (4)$$

In order to determine the objective function and to determine the scope of conducted research, a dimensional analysis was used. The symbols of Maxwell were used to describe the dimensions (length symbol L [m], mass symbol M [kg], time symbol T [s]).

The following is a matrix of dimensions created from exponents of dimension powers of accepted function arguments.

	D_y	k	Δh	L	d_{10}	υ	ρ_w
M	0	0	0	0	0	0	1
L	2	1	1	1	1	2	-3
T	-1	-1	0	0	0	-1	0

Selected three variables constituting the basis of the conducted analysis (k, I, d_{10}) were checked for dimensional independence. The determinant value which is different from zero is a necessary condition and sufficient dimensional independence of the adopted variables.

$$
\begin{array}{c|ccc}
 & \rho_w & d_{10} & k \\
\hline
M & 1 & 0 & 0 \\
L & -3 & 1 & 1 \\
T & 0 & 0 & -1
\end{array} = -1 \neq 0
$$

Hence, the dimensionless product of π_i of the spread of contaminants function can be represented in the following form:

$$\pi_1 = \rho_w^{a_1} d_{10}^{b_1} k^{c_1} D_y$$

$$\pi_2 = \rho_w^{a_2} d_{10}^{b_2} k^{c_2} \upsilon$$

$$\pi_3 = \rho_w^{a_3} d_{10}^{b_3} k^{c_3} L \qquad\qquad (5)$$

$$\pi_4 = \rho_w^{a_4} d_{10}^{b_4} k^{c_4} \Delta h$$

Below are the values of the searched exponents a_i, b_i, c_i for the product of dimensionless π_1.

$$(M^1 L^{-3}) a_1 (L^1) b_1 (L^1 T^{-1}) c_1 L^2 T^{-1} = M^0 L^0 T^0 \qquad\qquad (6)$$

From the equation of exponents, we obtained $a_i = 0$, $b_i = -1$, $c_i = -1$, thereby:

$$\pi_1 = \frac{D_y}{d_{10} k}. \qquad\qquad (7)$$

Form of the remaining dimensionless products is as follows:

$$\pi_2 = \frac{\upsilon}{d_{10} k},$$

$$\pi_3 = \frac{L}{d_{10}},$$

$$\pi_4 = \frac{\Delta h}{d_{10}}.$$

According to π's claim, the pre-established pollution spreading function can thus be replaced by:

$$f_1(D_y, k, \Delta h, L, d_{10}, \upsilon, \rho_w) = \Psi_1(\pi_1, \pi_2, \pi_3, \pi_4), \qquad\qquad (8)$$

where $\Psi_1(\pi_1, \pi_2, \pi_3, \pi_4)$ is a numerical function of the π_i dimensionless arguments.

The analysis allows the dependence of the D_y dispersion factor on four dimensionless π_i products. The phenomenon of pollutant spread in groundwater depends on the four dimensionless numbers obtained, as demonstrated by the dimensional analysis. In the experimental studies carried out, close interrelationships between the dimensionless products obtained were found.

6. DIMENSIONLESS PRACTICAL DEPENDENCIES OF DISPERSION COEFFICIENT D_Y

On the basis of the analysis of obtained dimensionless products and the review of dimensionless experimental dependencies, the following dependences were selected in terms of their practical application.
-   including Prandtl number and Reynolds number in form Pr = f(Re),
-   including Péclet number and Reynolds number in form Pe = f(Re).

To obtain the dependence of Pr = f(Re) the products of π_i were transformed in the form [10]:

$$\left.\begin{aligned}
\pi_1^* &= \frac{\pi_2}{\pi_1} = \frac{\upsilon}{D_y} = \text{Pr} \\[2em]
\pi_2^* &= \frac{\pi_4}{\pi_2 \pi_3} = \frac{k\, I\, d_{10}}{\upsilon} = \text{Re}
\end{aligned}\right\} \quad (9)$$

while in order to obtain the dependence of Pe = f(Re), the products of π_i were transformed into the following forms:

$$\left.\begin{aligned}
\pi_1^{**} &= \frac{\pi_4}{\pi_1 \pi_3} = \frac{k\, I\, d_{10}}{D_y} = \text{Pe} \\[2em]
\pi_2^* &= \frac{\pi_4}{\pi_2 \pi_3} = \frac{k\, I\, d_{10}}{\upsilon} = \text{Re}
\end{aligned}\right\} \quad (10)$$

The range of applied values of dimensionless numbers π_1^*, π_1^{**}, π_2^* is as follows:

$$8{,}00 \leq \pi_1^* \leq 39{,}71$$

$$0{,}65 \leq \pi_1^{**} \leq 3{,}43$$

$$0{,}02 \leq \pi_2^* \leq 0{,}43$$

Number π_2^* = Re contains hydraulic and physical parameters of the ground (k, I, d_{10}) used also in the dimension dependence determining the dispersion factor

D_y [2]. The values of π_2^* number corresponded to the range of laminar motion ($Re \leq 5$).
To determine the dependence of $\pi_1^* = f(\pi_2^*)$ an equation was developed in the form:

$$\pi_1^* = B_1 \pi_2^{*C_1} \tag{11}$$

while in order to determine the dependence of $\pi_1^{**} = f(\pi_2^*)$, the equation appears in the form:

$$\pi_1^{**} = B_2 \pi_2^{*C_2} \tag{12}$$

The values of dimensionless numbers together with the coefficients B_1, C_1, B_2 and C_2 (according to the least squares method) as well as the squares of deviations Δ^2 and the mean squared deviations include table no. 1 according to the relationships (11) and (12).

Table 1. The values of dimensionless numbers according to the relationships (11) and (12).

No.	π_1^*	π_1^* eq.	Δ^2	π_1^{**}	π_1^{**} eq.	Δ^2
1	2	3	4	5	6	7
1	39,7082	38,4439	1,5984	3,4315	3,2284	1,5784
2	33,3459	33,7773	0,1861	3,1524	3,0010	0,2461
3	26,8641	29,3252	6,0570	2,8558	2,8057	0,7016
4	26,8335	26,5647	0,0722	2,7597	2,6420	0,1714
5	23,3801	21,7759	2,5734	2,4279	2,7963	2,5464
6	23,0752	23,6132	0,2894	2,2236	2,4265	1,0031
7	22,3253	25,0936	7,6634	2,1753	2,1201	0,0894
8	21,5923	19,5197	4,2981	2,1716	2,3018	1,5264
9	20,0453	19,3447	0,4908	2,0040	2,0834	4,2663
10	19,8652	21,1282	1,5951	1,9098	1,8441	3,1109
11	18,6653	21,2893	6,8853	1,8427	1,9482	2,0652
12	16,8196	18,6167	3,2295	1,8224	1,8711	0,9416
13	16,8056	16,6693	0,0185	1,7383	1,7662	0,0427
14	16,6494	16,3404	0,0954	1,6536	1,6387	0,1723
15	16,5675	16,9828	0,1724	1,6257	1,7042	0,6461
16	16,1534	17,9093	3,0831	1,6045	1,5464	0,4772
17	15,6031	15,2651	0,1142	1,5694	1,6100	0,5227
18	15,3376	16,3021	0,9302	1,4953	1,4991	0,0431
19	14,7401	15,8518	1,2358	1,4512	1,4130	0,1793
20	14,3036	14,7747	0,2219	1,4067	1,4298	0,0964
21	14,0397	14,3813	0,1166	1,3842	1,3032	0,9445
22	13,0554	13,4088	0,1248	1,3781	1,4259	1,0332
23	12,9577	13,6959	0,5419	1,3622	1,2637	1,1331

24	12,1268	12,5435	0,1726	1,2869	1,2729	0,0391
25	11,7835	12,4345	0,4238	1,2090	1,2759	0,7733
26	11,6382	12,0676	0,1843	1,1861	1,1481	1,0428
27	10,9282	11,4130	0,2350	1,1657	1,1635	0,0095
28	10,5770	10,7742	0,0388	1,0704	1,0936	0,2982
29	10,1813	10,5779	0,1572	0,9962	0,9858	0,0378
30	9,5364	9,8352	0,0892	0,9816	1,0306	0,9193
31	9,2497	9,1885	0,0037	0,9173	0,8832	0,0970
32	9,0140	9,4060	0,1536	0,8546	0,8968	0,9495
33	8,7412	8,5361	0,0420	0,7545	0,7830	1,0016
34	8,6135	8,0625	0,3036	0,7069	0,6920	0,0058
35	8,0000	7,4437	0,3094	0,6510	0,6182	0,9091
	$B_1 = 4,8634$			$B_1 = 4,4433$		
	$C_1 = -0,5029$			$C_1 = 0,4707$		
	$\Delta = 1,1338$			$\Delta = 0,9298$		

7. SUMMARY, CONCLUSIONS AND INDICATIONS FOR FURTHER RESEARCH

In the course of the conducted analysis, it was proved that the coefficients of transverse dispersion D_y can be determined based on practical dimensionless relations (11) and (12) for the range of coarse sands.

When determining the size of D_y dispersion factors based on the dimensionless (11) and (12) relations in the following range of dimensionless products:

$$8,00 \leq \pi_1{}^* \leq 39,71$$

$$0,65 \leq \pi_1{}^{**} \leq 3,43$$

$$0,02 \leq \pi_2{}^* \leq 0,43$$

the error rates did not exceed 15%.

The analysis of dimensionless relations for determining the size of D_y transverse dispersion coefficients allows to determine the scope and amount of experimental investigations of the phenomenon of pollution spread in groundwater. It seems necessary for the further analysis of the conditions of modeling the spread of contaminants in groundwater to take into account cases of inhomogeneity and anisotropy of the soil medium, and to consider chemical and biological processes.

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WARUNKI MODELOWANIA FIZYCZNEGO ROZPRZESTRZENIANIA
ZANIECZYSZCZEŃ W WODZIE GRUNTOWEJ

Streszczenie

Praca zawiera przegląd bezwymiarowych zależności doświadczalnych określających współczynnik poprzecznej dyspersji Dy. W toku analizy wymiarowej zestawiono bezwymiarowe zależności doświadczalne opisujące rozprzestrzenianie zanieczyszczeń w wodzie gruntowej z parametrami hydraulicznymi i fizycznymi gruntu w przypadku ustalonego i jednostajnego ruchu wody gruntowej. Analiza pozwoliła na określenie bezwymiarowych zależności praktycznych określających współczynnik dyspersji w kierunku prostopadłym do głównego kierunku przepływu.

Słowa kluczowe: zanieczyszczenia, woda gruntowa, współczynnik dyspersji