



Estimation of the Vertical Diffusion Coefficient of Gas in Compacted Soils by Means of Mathematical Modeling

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Abstract. The density properties of subsiding loess soils were studied within the framework of mathematical modeling of their compaction using the method of deep explosions. Soil compaction is carried out to eliminate subsidence properties. Loess soils are characterized by low density and high porosity. The density properties of loess depend on the parameters of the diffusion interaction of gas atoms formed as a result of the explosion and the soil being compacted. Solving inverse applied problems that arise when studying mathematical models of geological systems allows us to systematize knowledge about them. The work considers the inverse problem of estimating the diffusion coefficient. Mathematical modeling of the vertical diffusion coefficient in anisotropic and isotropic geological systems was carried out. The case of complete absorption of gas atoms by the surrounding soil has been studied. A numerical assessment of the coefficient of vertical diffusion in soil before and after compaction has been implemented, over time and with an accuracy sufficient for engineering calculations. Gas diffusion coefficients in soils of various densities were obtained. The constructed mathematical relationships for estimating the coefficient of vertical diffusion make it possible to predict the density properties of soils at the stage of designing the foundations of construction projects.

Keywords: mathematical modeling; numerical assessment; computational experiment; subsidence; soil compaction; diffusion coefficient.

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Оценка коэффициента вертикальной диффузии газа в уплотняемых грунтах средствами математического моделирования

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Аннотация. Исследованы плотностные свойства просадочных лёссовых грунтов в рамках математического моделирования их уплотнения методом глубинных взрывов. Уплотнение грунтов производится для исключения свойства просадочности. Лёссовым грунтам характерна низкая плотность и высокая пористость. Плотностные свойства лёссов зависят от параметров диффузионного взаимодействия атомов газа, образующегося в результате взрыва, и уплотняемого грунта. Решение обратных прикладных задач, возникающих при исследовании математических моделей геологических систем, позволяет систематизировать знания о них. В работе рассмотрена обратная задача об оценке коэффициента диффузии. Проведено математическое моделирование коэффициента вертикальной диффузии в анизотропных и изотропных геологических системах. Исследован случай полного поглощения атомов газа окружающим его грунтом. Реализована численная оценка коэффициента вертикальной диффузии в грунте до и после его уплотнения, с течением времени и точностью достаточной для инженерных расчётов. Получены коэффициенты диффузии газа в грунтах различной плотности. Построенные математические соотношения оценки коэффициента вертикальной диффузии позволяют прогнозировать плотностные свойства грунтов на этапе проектирования оснований и фундаментов строительных объектов.

Ключевые слова: математическое моделирование; численная оценка; вычислительный эксперимент; просадочность; уплотнение грунта; коэффициент диффузии.

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1. Introduction

The design of buildings and civil engineering structures is accompanied by numerical calculations of the density and deformation characteristics of subsiding loess soil. Loess is quite mysterious; on a planetary scale, it is a rock of the Quaternary period [1], [2]. Loess is characterized by a yellow, yellow-brown or yellow-fawn color [3]–[6]. They have high porosity and low density [7].

Methods for eliminating subsidence are varied and depend on the conditions of implementation [8]. We are exploring the method of soil compaction by explosion, which in the process of practical implementation shows high economic efficiency at low production costs [9], [10]. Within the framework of mathematical modeling of the compaction of subsidence soils, studies of their individual strength and deformation properties have been carried out [11]–[13]. Interpretation of soil strength characteristics for numerical studies was carried out in [14], [15]. When compacted by explosion, soils are subject to dynamic loads [16], [17]. Within the framework of mathematical modeling of the compaction of subsidence soils, the dependence of the density properties of loess on the parameters of the diffusion interaction of gas and soil atoms is traced.

For a comprehensive description of the mathematical model of compaction of subsidence soils by explosion, additional scientific research and the solution of individual inverse problems are required. One of which determines the purpose of the article - modeling the coefficient of vertical diffusion in anisotropic and isotropic compacted geological systems with complete absorption of gas atoms

by the surrounding soil. To achieve the goal, this article describes the solution of the following problems: the results of mathematical modeling of the density of subsidence soils during their compaction by deep explosions; development of a solution to the inverse problem of estimating the coefficient of vertical diffusion in soils of various densities using numerical modeling methods; implementation of a software computational experiment with an accuracy sufficient for engineering calculations.

2. Mathematical model of compaction of subsidence soils

The mathematical model of compaction of subsidence soils by the explosion of a concentrated explosive charge is described by a parabolic equation of the form [11]

$$\frac{\partial q}{\partial t} + U \frac{\partial q}{\partial x} = \frac{\partial}{\partial x} K_x \frac{\partial q}{\partial x} + \frac{\partial}{\partial y} K_y \frac{\partial q}{\partial y} + \frac{\partial}{\partial z} K_z \frac{\partial q}{\partial z} + f, \quad t \in [t_0, T], \quad (1)$$

with initial condition

$$q(t_0, x, y, z) = Q \delta(x - x^0) \delta(y - y^0) \delta(z - z^0) \quad (2)$$

and boundary condition

$$q(t, x, y, z) \Big|_{z=z^0} = 0, \quad t > t_0, \quad (3)$$

where $Q = \text{const} > 0$ – power of the explosive charge, $\delta(x)$ – Dirac delta function, $z^0 = H$ – depth of placement of the concentrated explosive charge, $U = \text{const}$ – speed of horizontal transfer (along the Ox axis), q – average soil density, K_x, K_y, K_z – diffusion coefficients.

The initial boundary value problem (1)–(3) characterizes changes in the values of the average density of the compacted soil skeleton per unit time t at point (x, y, z) . Boundary condition (3) corresponds to the case of complete absorption of gas atoms released during an explosion by the surrounding soil. In this case, compaction of subsidence soil is realized [11].

Let us represent the function of the explosive gas source in the form

$$f(t, x, y, z) = Q \cdot R(t, x, y, z) = Q \delta(t - t_0) \delta(x - x^0) \delta(y - y^0) \delta(z - H).$$

Let us assume that U, K_x, K_y, K_z are continuous functions of the argument z :

$$U = U(z), \quad K_x = K_x(z), \quad K_y = K_y(z), \quad K_z = K_z(z).$$

The solution to problem (1)–(3) for calculating the average values of the density of the compacted soil skeleton is determined by the relation [13].

$$\begin{aligned} q(t, x, y, z) = & \frac{Q}{(2\pi)^{3/2} \sigma_x \sigma_y \sigma_z t^3} \times \\ & \times \exp \left\{ - \left(\frac{(x - \bar{U}t)^2}{2\sigma_x^2 t} + \frac{y^2}{2\sigma_y^2 t} \right) \right\} \times \\ & \times \left[\exp \left\{ - \frac{(z - H)^2}{2\sigma_z^2 t} \right\} - \exp \left\{ - \frac{(z + H)^2}{2\sigma_z^2 t} \right\} \right], \end{aligned} \quad (4)$$

which is a function of the density distribution of the soil skeleton, where $\sigma_x^2(t), \sigma_y^2(t), \sigma_z^2(t)$ – dispersion coordinate changes of gas atoms in the compacted soil, respectively, along the Ox, Oy, Oz axes at time t ; $\sigma_x^2(t), \sigma_y^2(t), \sigma_z^2(t)$ – functions continuously differentiable with respect to the time argument $t, t \geq 0$.

3. Vertical diffusion coefficient modeling

Estimating the diffusion coefficient of gas atoms released during the explosion of a concentrated explosive charge is an inverse problem within the framework of mathematical modeling of the compaction of subsidence soils.

Statement of the inverse problem. According to the known average values of the density of the soil skeleton $q(t, x, y, z)$, compacted by the method of deep explosion of a concentrated source of explosive, provided that the gas is completely absorbed by the surrounding soil (compaction of subsidence soil), as well as according to a given depth of placement of the explosive H and known values of charge power Q of the explosive, determine the values $\sigma_z^2(t)$ – vertical dispersion of the coordinates of gas atoms in the compacted soil along the Oz axis at time t . Estimate the vertical diffusion coefficient K_z over time and with a given accuracy.

Let us carry out numerical modeling and construct an approximate solution to the posed inverse problem based on the apparatus of numerical methods for solving transcendental equations [17], [18].

The solution of the problem for the case of complete absorption of gas atoms by the surrounding soil (implementation of compaction of the subsidence layer) will be carried out using a simple iteration method. Assuming that the interval $[a, b]$ is separated (we will estimate a and b by the selection method or graphically), containing the required root σ_z equations

$$\begin{aligned} q(t, x, y, z) = & \frac{Q}{(2\pi)^{3/2} \sigma_x \sigma_y \sigma_z t^3} \times \\ & \times \exp \left\{ - \left(\frac{(x - \bar{U}t)^2}{2\sigma_x^2 t} + \frac{y^2}{2\sigma_y^2 t} \right) \right\} \times \\ & \times \left[\exp \left\{ - \frac{(z - H)^2}{2\sigma_z^2 t} \right\} - \exp \left\{ - \frac{(z + H)^2}{2\sigma_z^2 t} \right\} \right] = 0. \end{aligned} \quad (5)$$

Taking into account that the geological environment under study has characteristic properties of anisotropy, we transform equation (5) to the form:

$$\begin{aligned} \sigma_z = & \frac{Q}{q(t, x, y, z) (2\pi)^{3/2} \sigma_x \sigma_y t^3} \times \\ & \times \exp \left\{ - \left(\frac{(x - \bar{U}t)^2}{2\sigma_x^2 t} + \frac{y^2}{2\sigma_y^2 t} \right) \right\} \times \\ & \times \left[\exp \left\{ - \frac{(z - H)^2}{2\sigma_z^2 t} \right\} - \exp \left\{ - \frac{(z + H)^2}{2\sigma_z^2 t} \right\} \right]. \end{aligned}$$

The iterative process of successive approximations to the desired root will be numerically determined by the formula

$$\begin{aligned} \sigma_z^{(n+1)} = & \frac{Q}{q(t, x, y, z)(2\pi)^{3/2} \sigma_x \sigma_y t^3} \times \\ & \times \exp \left\{ - \left(\frac{(x - \bar{U}t)^2}{2\sigma_x^2 t} + \frac{y^2}{2\sigma_y^2 t} \right) \right\} \times \\ & \times \left[\exp \left\{ - \frac{(z - H)^2}{2(\sigma_z^{(n)})^2 t} \right\} - \exp \left\{ - \frac{(z + H)^2}{2(\sigma_z^{(n)})^2 t} \right\} \right]. \end{aligned} \quad (6)$$

If the geological environment under study has characteristic isotropic properties, then $\sigma_z = \sigma_y = \sigma_x$. Therefore, equation (5) can be transformed to the form

$$\begin{aligned} \sigma_z = & \sqrt[3]{\frac{Q}{q_2(t, x, y, z)(2\pi)^{3/2} \sigma_z^2 t^3}} \times \\ & \times \sqrt[3]{\exp \left\{ - \left(\frac{(x - \bar{U}t)^2}{2\sigma_z^2 t} + \frac{y^2}{2\sigma_z^2 t} \right) \right\}} \times \\ & \times \sqrt[3]{\left[\exp \left\{ - \frac{(z - H)^2}{2\sigma_z^2 t} \right\} - \exp \left\{ - \frac{(z + H)^2}{2\sigma_z^2 t} \right\} \right]}. \end{aligned}$$

Instead of (6), we will construct an iterative sequence of approximations to the desired root using the formula

$$\begin{aligned} \sigma_z^{(n+1)} = & \sqrt[3]{\frac{Q}{q_2(t, x, y, z)(2\pi)^{3/2} (\sigma_z^{(n)})^2 t^3}} \times \\ & \times \sqrt[3]{\exp \left\{ - \left(\frac{(x - \bar{U}t)^2}{2(\sigma_z^{(n)})^2 t} + \frac{y^2}{2(\sigma_z^{(n)})^2 t} \right) \right\}} \times \\ & \times \sqrt[3]{\left[\exp \left\{ - \frac{(z - H)^2}{2(\sigma_z^{(n)})^2 t} \right\} - \exp \left\{ - \frac{(z + H)^2}{2(\sigma_z^{(n)})^2 t} \right\} \right]}. \end{aligned} \quad (7)$$

The first approximation of $\sigma_z^{(1)}$ to the desired root (first iteration) is taken to be any value of σ_z , belonging to a segment of root division $[a, b]$.

The criterion for completing the computational process of searching for a numerical solution to equation (5) is the fulfillment of the inequality

$$|\sigma_z^{(n)} - \sigma_z^{(n-1)}| < \varepsilon,$$

where ε is the accuracy of calculations

The dispersion of coordinate changes of gas atoms is related to the vertical diffusion coefficient by the relation

$$\sigma_z^2 = \frac{2}{h} \int_0^h K_z(z) dz, \quad (8)$$

where h is the depth of penetration of gas atoms into the surrounding soil.

4. Computing experiment

Numerical modeling of the diffusion coefficient of gas formed as a result of an explosion into the surrounding soil is carried out using the example of soil in the city of Budennovsk, Stavropol Territory. According to the engineering-geological structure, the territory of Budennovsk is considered the “capital” of subsidence soils of the world. The main element of the engineering-geological section of the city is loess and loess-like loams with a thickness of up to 40 m, in the Budennovsky district - up to 100 m. The next element of the section is composed of clays with layers of sand, occurring at depths from 10 to 70 m, and with a thickness of up to 30 m [20].

Before constructing buildings and structures on loess soils, preliminary compaction is required. One of the low-cost and effective methods is the compaction of a concentrated explosive charge by explosion. During a deep explosion of industrial explosives, gases (mainly carbon and nitrogen oxides) are released into the surrounding soil [21].

To estimate the gas diffusion coefficient in soil based on iterative processes (6), (7) and relation (8), a program was developed in the Python programming language [22]. It is designed to calculate the values of vertical diffusion coefficients over time and with an accuracy sufficient for engineering calculations.

Fig. 1 shows a graphical interpretation of the vertical diffusion coefficient when compacting loess with a density of 1.5 g/cm³ by explosion. Explosive charge power 5 kg. Its depth is 6 m. The initial data of the computational experiment are taken from the design documentation of the object “Stavropoln”, Budennovsk [9].

Analysis of the values presented in Fig. 1 showed that the vertical diffusion coefficient reaches its maximum value of 0.60608 cm²/s at the moment of the explosion. Then it decreases over time. This is due to the type of gas source; it is concentrated and instantaneous.

Three months after draining the pit, 5 wells were drilled to sample monoliths. The density of the soil compacted by the explosion averaged 1.7 g/cm³ [9]. Tabl. 1 shows the values of soil diffusion coefficients over time, calculated according to the iterative process (6) and relation (8).

A graphical interpretation of the result of the experiment to estimate the coefficient of vertical diffusion of gas in soils of various densities is shown in Fig. 2.

The value of the coefficient of vertical gas diffusion in soil with a density of 1.5 g/cm³ is higher than with a soil density of 1.7 g/cm³. The diffusion coefficient decreases by up to 13%.

Numerical modeling of the diffusion coefficient for various soils in the city of Budennovsk was carried out. Fig. 3 shows the implementation of modeling the dynamics of its change for loess, sand, sandy loam, loam and clay. The maximum value of the vertical diffusion coefficient of 0.60608 cm²/s is recorded for loess. Moreover, its minimum value is 0.46621 cm²/s for clay. Over time, after 1 s, the diffusion coefficient takes on a value of 0.03 cm²/s with an accuracy of 0.01, sufficient for engineering calculations.

5. Conclusion

The result of the study is a numerical assessment of the coefficient of vertical diffusion of gas in soil within the framework of mathematical modeling of its compaction by explosion. A case of complete absorption of gas atoms by the surrounding soil during compaction is described. The isotropic and anisotropic properties of the compacted soil are taken into account. The compiled mathematical

expressions make it possible to carry out computational experiments with the required accuracy. Gas diffusion coefficients in soils of various densities were obtained.

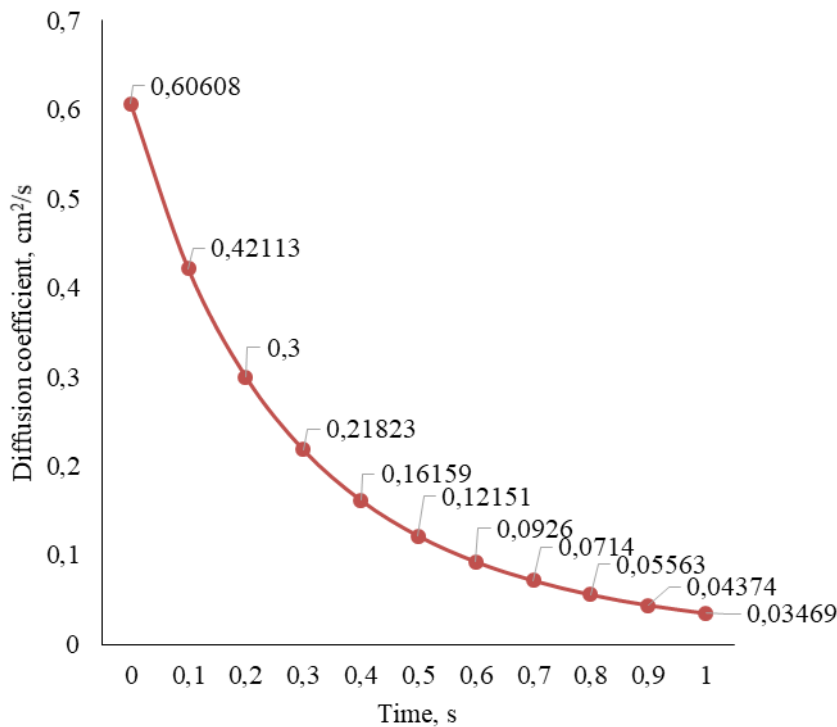


Fig.1. Values of the vertical diffusion coefficient of gas in soil over time.

Table 1. Vertical diffusion coefficient before and after soil compaction by explosion.

Time	Diffusion coefficient	
	before compaction	after compaction
0.0	0.6060	0.5347
0.1	0.4211	0.3715
0.2	0.3000	0.2647
0.3	0.2182	0.1925
0.4	0.1615	0.1425
0.5	0.1215	0.1072
0.6	0.0926	0.0817
0.7	0.0714	0.0630
0.8	0.0556	0.0490
0.9	0.0437	0.0386
1.0	0.0346	0.0306

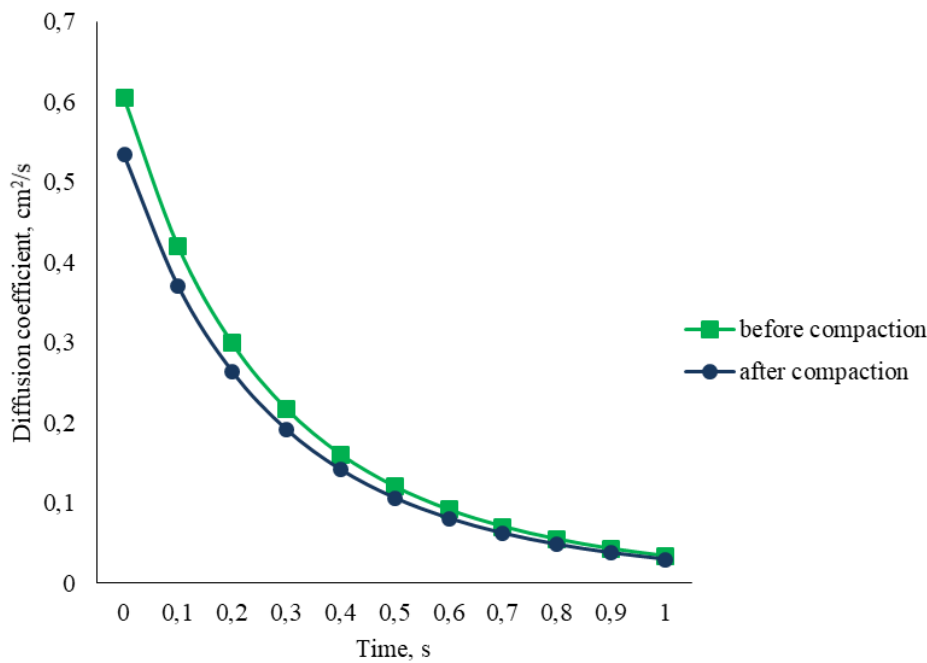


Fig.2. Values of coefficients of vertical diffusion of gas in soil over time before and after compaction by explosion.

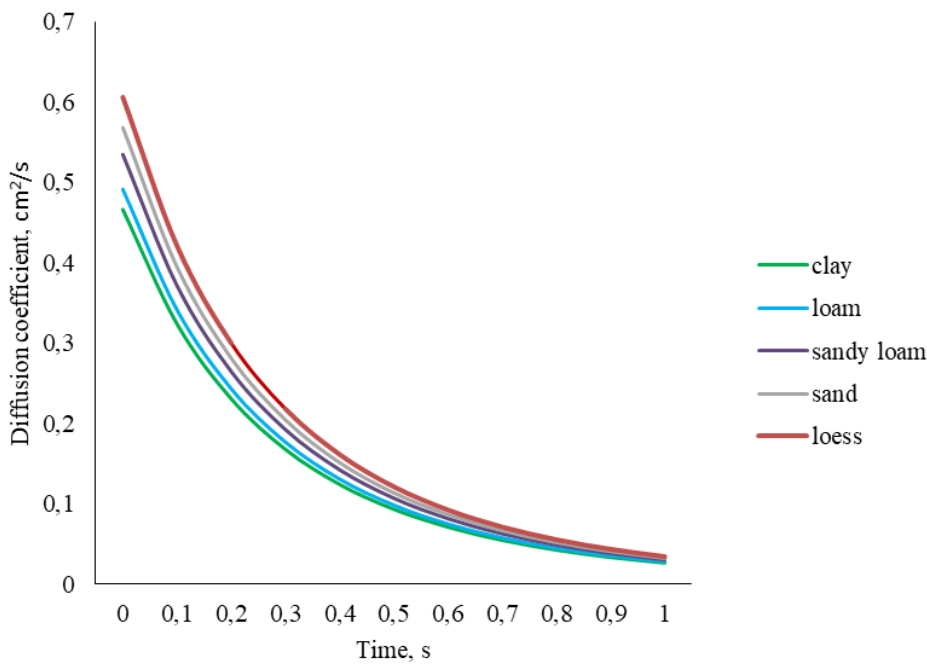


Fig.3. Values of coefficients of vertical diffusion of gas in soil over time before and after compaction by explosion.

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