Technical Report

Risk Assessment for Alkaline Water Outflow from Iron and Steel Slag Using the pH Simulation Technique

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Abstract

Iron & Steel Slag has properties such as high strength and bearing capacity as geo-material, has been used for low cost pavement such as temporary work road and storage yard etc. other than roadbed aggregate. On the other hand, slag is alkaline, so consideration or countermeasure for outflow of alkali water is very important. Long term risk simulation on diffusion of alkaline is conducted with convective dispersion analysis considering mechanical and alkali elution property of slag, adsorption property of surrounding soil.

1. Introduction

Iron and steel slag is a granular material that can be well compacted for large bearing capacities, and can be used not only as a sub-base course material (JIS A 5015) for road construction but also for temporary work roads, storage yards pavement, etc. on weak subsoils. Conversely, when slag is used as an uncovered pavement, appropriate measures are necessary to prevent the alkalized rainwater outflow from the slag. Therefore, the alkali risk assessment in slag application for civil engineering works on land by numerical simulation based on an existing program for convective dispersion analysis was performed, with due consideration given to the physical properties of slag, the elution of alkalis (elute flux) from slag, and the alkali adsorption of the surrounding soil.

2. Outline of the Analysis

The extent of the influence of alkali was simulated using the three-dimensional (3D) convective dispersion analysis program G-TRAN/3D¹⁾ in which a "seepage flow analysis simulates the flow of water" and a "convective dispersion analysis simulates the flow of substance." The flow of analysis and the basic theory of the program used are described below.

2.1 Flow of analysis

In the seepage flow equation, which is described later, seepage and convective dispersion can be handled separately as a different phenomenon assuming that the change in solute concentration in fluid does not cause any change in fluid density. In the simulations, the pressure and flow velocity distribution of water in ground are initially calculated by seepage flow analysis. Next, the concentration distribution of a chemical substance that flows as per the flow velocity distribution is calculated by convective dispersion analysis. **2.2 Governing equation and parameters used in each analysis** 2.2.1 Seepage flow analysis

The equation used in seepage flow analysis is shown below (Equation 1). Assuming that there are no density currents, the equation can be derived from the law of conservation of mass and Darcy's law (i.e., the relationship between water head and flow velocity) for the fluid flowing through soil microelements.

$$\frac{\partial}{\partial x_{i}} \left(\rho K_{r} K_{ij}^{s} \frac{\partial \varphi}{\partial x_{j}} + \rho K_{r} K_{i3}^{s} \right) + \rho q = \rho \left(\beta S_{s} + C_{s} \right) \frac{\partial \varphi}{\partial t}$$
(1)

where ρ is the fluid density, K_r is the tensor of the ratio of unsaturated hydraulic conductivity to saturated hydraulic conductivity, and K_{ij}^{s} is the tensor of saturated hydraulic conductivity, which is represented as follows:

$$K_{ij}^{s} = \begin{bmatrix} k_{11} & k_{12} & k_{13} \\ k_{21} & k_{22} & k_{23} \\ k_{31} & k_{32} & k_{33} \end{bmatrix}$$
(2)

where *i*, *j* = 1, 2, 3 (1: *x*, 2: *y*, 3: *z*; *xyz* components of orthogonal coordinates); K_{i3}^{s} are the parts related to the *z* direction in the tensor of saturated hydraulic conductivity, i.e., k_{13} , k_{23} , and k_{33} ; φ is the total head; *q* is the amount of inflow or outflow; S_s is the specific storage coefficient; β is the coefficient indicating whether specific storage coefficient is valid ($\beta = 1$ for saturated and 0 for unsaturated); and C_s is the specific water capacity.

The parameter specific storage coefficient S_s is required for evaluating the unsteady groundwater flow, which indicates the quantity

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of water extracted from a unit value pore when the unit drop of water level occurs.

The ratio specific water capacity $d\theta/d\varphi$ is the variation in volume water content θ with the water head φ .

For the water retention curve (or soil–water characteristic curve), the empirical formula²⁾ of van Genuchten (VG) is shown below.

$$S_e\left(=\frac{\theta}{n}\right) = \left(\frac{1}{1+(\alpha\varphi)^n}\right)^{1-1/n}$$
(3)

where S_e is the effective saturation degree, *n* is porosity, and α and *n* are the VG parameters.

The specific permeability coefficient, which is the ratio of unsaturated hydraulic conductivity to saturated hydraulic conductivity, is expressed as follows:²⁾

$$k_{r} = \frac{k_{ij}}{k_{ij}^{s}} = Se^{\frac{1}{2}} \left[1 - \left(1 - Se^{\frac{1}{m}} \right)^{m} \right]^{2}$$
$$m = 1 - \frac{1}{n}$$
(4)

where *m* and *n* are the constants.

2.2.2 Convective dispersion analysis

The equation used for convective dispersion analysis is shown below (Equation 5^{3}). The substance of concern in convective dispersion analysis is the hydroxyl ion [OH⁻].

$$R\theta\rho\frac{\partial c}{\partial t} = \frac{\partial}{\partial x_i} \left(\theta\rho D_{ij}\frac{\partial c}{\partial x_j}\right) - \theta\rho V_i\frac{\partial c}{\partial x_i} - R\theta\rho\lambda c - Q_c$$
(5)

where *R* is the delay coefficient, θ is the volume water content, ρ is the fluid density, D_{ij} is the dispersion tensor, *C* is the concentration, V_i is the flow velocity through the pore, λ is the damping coefficient, and Q_c is the term of source.

The dispersion tensor is expressed by Bear as follows: 4)

$$D_{ij} = \alpha_t \|v\| \delta_{ij} + (\alpha_L - \alpha_T) \frac{v_i v_j}{\|v\|} + D_m \tau \delta_{ij}$$
(6)

where α_L is the longitudinal dispersion length, α_T is the transverse dispersion length, v_i is the vector of flow velocity through the pore, D_m is the molecular diffusion coefficient, τ is the labyrinth factor, ||V|| is the absolute value of actual flow velocity, and δ_{ij} is the Kronecker delta (1: when i = j and 0: when $j \neq j$).

The fluid flow velocity is generally higher than the molecular diffusion rate such that the influence of the molecular dispersion is negligible. The longitudinal and transverse dispersion lengths express the extent of concentration distribution due to the uniformity of flow velocity of water, the pore distribution, and the size. In the convective dispersion equation, they are handled as the dispersion tensor according to the assumption that the abovementioned phenomenon is equivalent to the phenomenon of substance diffusion caused by a difference in concentration. The length of dispersion in the direction of flow velocity is called longitudinal dispersion length, and that in the direction perpendicular to the direction of flow velocity defined transverse dispersion length. It has been reported that the dispersion length is proportional to the groundwater flow velocity.⁵⁾ Thus, the transverse dispersion length.

From the results of in situ tracer tests, it is known that the dispersion length has a tendency to depend on the test scale, and then the longitudinal dispersion length was considered from 1/100 to 1/1 of the moving distance of the substance.^{6, 7)}

The labyrinth factor τ is the correction term for adapting the molecular dispersion coefficient in a porous medium as the effective molecular dispersion coefficient, which is calculated as the ratio of straight flow passage length L to actual flow passage length $L_{a}^{.8}$

$$\tau = \left(\frac{L}{L_e}\right)^2 \tag{7}$$

In this case, the labyrinth factor is less than 1. It is generally considered to be from 0.3 to 0.64.⁹⁾

Adsorption includes the action where the solute sticks to the surface of soil particles through chemical adsorption, sorption, ion exchange, etc. It helps to retard the movement of the substance. The groundwater flow velocity is usually lower than the reaction rate and is evaluated using the linear adsorption model. In the case of linear adsorption, the amount of adsorption is assumed to be proportional to the concentration of solution, and is expressed by the following equation:

$$C' = k_d c \tag{8}$$

where C' is the amount of adsorption per unit dry weight of soil particle, k_d is the distribution coefficient, and c is the liquid concentration.

For the linear adsorption model, the relationship between distribution coefficient k_d and the retardation coefficient R is given by the following equation:

$$R = 1 + \frac{\theta}{\rho} k_d \tag{9}$$

where, R is the retardation coefficient, k_d is the distribution coefficient for a saturated soil, ρ_d is the dry density of the soil, and θ is the volume water content.

Distribution coefficient k_d is the concentration ratio between two different phases (i.e., soil and pore water in the present discussion) that are in contact with each other and are in an equilibrium state, which can be obtained by a serial batch test. In particular, when handling a problem with alkali, mixtures of the soil and solution (calcium hydroxide solution) is first prepared by changing the weight of soil and the concentration of calcium hydroxide solution. Next the mixtures were shaken. From the changes in pH of the solutions after shaking, the distribution coefficient can be obtained from the gradient in the relationship between concentration of solution and amount of alkali adsorption of soil in the equilibrium state after adsorption (**Fig. 1**).

When the solution concentration in an adsorption equilibrium state increases to a certain level (Fig. 1), the alkali adsorption per unit weight of soil becomes invariable. The alkali adsorption per unit weight of soil at this point is defined the alkali adsorption capacity.



Fig. 1 Example of relation of concentration [OH⁻] of liquid phase and OH⁻ absorbed by soil particles in equilibrium by alkali absorption test

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Conversely, the distribution coefficient k_d also varies as per the solution concentration in the equilibrium state after alkali adsorption. That is, it decreases as the solution concentration increases. The retardation coefficient, R, is equal to or greater than 1. When R = 1, alkali adsorption does not occur at all.

When the cumulative concentration of adsorbed alkali reaches the alkali adsorption capacity, the following calculations are performed assuming that $k_d = 0$ and R = 1, that is, the adsorption of alkali does not occur anymore.

The source term Q_i indicates the flux of the substance from slag, which is given as an exponential function or fixed concentration (e.g., pH).

Neither the seepage flow nor convective dispersion equations both expressed in the form of partial differentiation—can be directly applied to solve problems involving a soil configuration of a complicated shape. Therefore, the seepage flow equation is approximated and discretized by finite element method using Galerkin method as one of weight residual method which applies shape function as the weight function. In the case of the convective dispersion equation, convection and dispersion are separated by the Eulerian-Lagragian Numerical Metod and formulated using the FEM. For further details, refer to the references.^{3, 10)}

3. Example of Analysis using the pH Simulation Technique

3.1 Outline of the simulation model

Figure 2 shows the simulation model. It comprises an uncovered temporary sub-base course of iron and steel slag that is 5 m wide and 0.25 m thick and a uniform subgrade of humus and clayey soil. To avoid undesirable dimensional effects, ample allowance was given to the subgrade dimensions (50 m deep and 1000 m wide). The annual rainfall was assumed to be 1800 mm, and 50% of the rainfall was assumed to permeate in the slag layer and flow in the subgrade. For a simulation period of 100 years, the calculation was performed daily, in which the annual rainfall converted into the average daily rainfall was stored continuously in the model for convenience. Though the rainwater infiltration in the slag layer with long-term solidification, the permeability coefficient was assumed to remain the same.

No assumptions were made concerning the subgrade groundwater level. In fact, a natural flow of groundwater was caused by seepage flow analysis, in which the right-hand side (downstream side) of the model was assumed to be the seepage surface, and the left-hand side (upstream side) and bottom of the model were assumed to be impermeable boundaries.



Fig. 2 Simulation model

Table 1 Simulation parameter

		Slag	Ground
Application site		Pavement	Original
			ground
Particle density (g/cm ³)		3.3	2.7
Porosity ratio N		0.5	0.5
Coefficient of permeability (cm/s)		5×10 ⁻³	1×10 ⁻⁴
Longitudinal dispersion length (m)		0.5	0.5
Transverse dispersion length (m)		0.05	0.05
	0 year	12.3	7
Alkali elute property	10 year	10	_
(pH of void water)	50 year	11.8	_
	100 year	11.7	-
Maximum ability of alkali absorption		-	1.0×10^{-3}
(OH ⁻ mol/g)			1.0^10 *

Table 1 lists the simulation parameters. Almost all the soil parameters shown here are the default values of the simulation program. Among the alkali adsorption characteristics, the data of distribution coefficient was given for each representative solution concentrations in an equilibrium state obtained by a batch test using a soil having nearly the same alkali adsorption capacity (maximum alkali adsorption $\mathrm{C}_{_{\mathrm{max}}})$ as the simulation model. The VG parameter, as the moisture characteristic of slag, was obtained using the soil column method,¹¹⁾ in which water is passed through a cylinder filled with the slag, and the moisture content of the slag in the direction of height after the cylinder is left for one day is measured and fitted using the VG model. The elution characteristic of the slag was obtained by continuously pouring distilled water over a column filled with the slag, measuring the change in the pH of infiltration, and determining the relationship between the cumulative poured liquid to solid ratio (i.e., the ratio of cumulative water poured over the column to the slag weight) obtained by the experiment and the measured pH value. The cumulative flowed liquid to solid ratio in experiment transformed to elapsed years in situ as the cumulative flowed liquid to solid ratio in experiment is accorded with that in situ (rainwater infiltration amount \times elapsed years/(slag thickness \times density)).

As one of the results of the seepage flow analysis, the groundwater flow velocity vector in steady state is shown in **Fig. 3**. It can be seen from the figure that the vector straight downward is predominant and that the surface of groundwater has been formed in the original ground layer at a considerably low level.

Using the abovementioned flow velocity vector, a convective dispersion analysis was performed to estimate the concentration of OH^- in pore water in the lower layer of the slag after 100 years. The distribution of OH^- concentration converted in terms of pH is shown in **Fig. 4**. From the figure, OH^- ions were largely dispersed in the



Fig. 3 Result of infiltration flow analysis –distribution of the velocity of a flowing in ground at ateady atate–

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Fig. 4 Result of convective diffusion analysis –distribution of pH of pore water in ground after 100 year–

vertical direction, and the largest depth of dispersion was approximately 0.75 m. Conversely, OH⁻ ions were also dispersed horizontally, though less conspicuously. This is because of the influence of groundwater flow. In this case, the depth was approximately 0.2 m downstream from the foot of the slag slope.

In the present simulation, not only the decrease in rainwater infiltration due to a decline in permeability coefficient of the slag layer but also the influence of carbonization, the neutralization of carbon dioxide in soil, etc. were not considered so that the simulation results obtained are considered to be realistic. Nonetheless, the abovementioned uncertain factors need to be investigated in the future.

4. Conclusion

We consider that the pH simulation technique presented in this study is useful in assessing the risk of alkali water elution and the measures taken to avoid the risk when using iron and steel slag in civil engineering works on land. In the future, we would like to improve the accuracy of the simulation by validating the simulation results against the actual in situ dates on alkali diffusion in the surrounding ground around the slag and then to ensure the safety of the elution of alkali when iron and steel slag is used for civil engineering works on land.

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