Research on the Contaminant Breakthrough Time Algorithm Based on Thermal Penetration Theory

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This work was supported in part by the Open Research Fund Program of the State Key Laboratory of Hydrosience and Engineering, Tsinghua University under Grant sklhsse-2020-D-06 and in part by the National Key R & D Program of China under Grant 2018YFC1802700.

ABSTRACT The current calculation method of breakthrough time calculates the concentration value of the measuring point at different times based on the model solution, which is determined by approaching the concentration value corresponding to the breakthrough standard through trial calculations. However, it is necessary to research the breakthrough standard with practical applications of mathematical and physical significance, especially a one-dimensional mathematical model of contaminant migration under Dirichlet boundary conditions. A general algorithm for directly calculating the breakthrough time was established in this research. Moreover, the calculation standard of the breakthrough time was also discussed based on the similarity between the analytical solution and the mathematical law of thermal conduction. This research considered parameters of the seepage velocity, dispersion coefficient and characteristics of the impervious layer, and the sensitivity analysis of these factors were investigated. The results show that the proposed algorithm was basically consistent with the current method, and the concept of thermal penetration depth is also feasible for the calculation standard. This is not only suitable for different breakthrough standards, but also simple and convenient. This study can provide a reference for the design, management and subsequent remediation of actual sites.

INDEX TERMS Breakthrough time, mathematical model, convection dispersion, analytical solution, general algorithm.

I. INTRODUCTION

Landfills are the most widely used and important sites for treating urban solid waste [1-4]. To reduce the groundwater contamination caused by leachate migration in landfills, the compacted clay liners [5] and geomembranes [6] have been widely used as the bottom liners of landfills. However, under the long-term action of leachates, contaminants can still enter the environment through the landfill liner, resulting in a potential threat to groundwater and soil [7, 8]. Therefore, evaluating the invalid time of seepage materials is a critical task in the design, operation and management of landfills.

For anti-seepage materials, the breakthrough time is generally used to evaluate their invalid time [9], and extensive research has made many major breakthroughs in basic theory and engineering practice. For example, to predict the service life of a landfill, the migration of four contaminants in five landfills was simulated by considering the contaminant and concentration flux perspectives [10]. In other research, 1% of the initial contaminant concentration [11] or 5% of the stable downstream flux [12] was taken as the breakthrough time standard. The time required for contaminants to penetrate the barrier and reach the standard concentration threshold is called the breakthrough time in the basic theory of environmental geotechnical technology; in addition, 10% of the initial concentration is the standard when determining the breakthrough time [12]. For the above research, the definition has relative properties that depend on the percentage of the downstream and upstream contaminants.
However, the threshold concentration in the groundwater quality standard is also considered to be the breakthrough standard when the first contaminant is detected downstream [14]; moreover, the ratio of the limit value in drinking water and the concentration value of contaminant is taken as the breakthrough standard, and the typical breakthrough standard and the extreme breakthrough standard have been proposed [15]. Other studies have taken cadmium and dichloroxylene as representative contaminants and take the US maximum contaminant level (MCL) as the standard [16] or study different contaminants and different breakthrough threshold concentrations as indicators [17] when the contaminant passes the landfill barrier system. The above studies used different contaminants or standards to define the breakthrough time according to the actual problems. However, the concept of breakthrough time has different interpretations due to the complexity and variability of the actual problems. Thus, it is difficult to directly compare the different calculation results of application examples that reflect the anti-seepage effect of landfill barriers.

The current calculation method for the breakthrough time algorithm is divided into two categories. The first builds a mathematical model based on actual examples, which focuses on the numerical solution method [18-20]. For example, the breakthrough time is calculated using a numerical method under different conditions for the design of seepage curtain thickness [13], and the finite element method is commonly used by establishing a grid model and defining the initial and boundary conditions, but the calculation process is usually time-consuming and complex [21, 22]. In the second approach, an analytical solution is given by constructing the initial and boundary conditions of the mathematical model based on a one-dimensional convective dispersion equation [13, 15, 23, 24]. However, the traditional mathematical analysis method of solving partial differential equations is also very complex [25, 26], and it is more complicated in engineering applications as a result of the difficulty and cost of anti-seepage layer design and management. In the above studies, the calculation method of breakthrough time was relatively complicated by the numerical method or the analytical method, because the model solutions were mainly based on gradual trial calculation steps. Therefore, a basic theoretical approach should seek a simplified calculation method for different penetration velocities and anti-seepage layer characteristics.

The purpose of this study is to discuss the mathematical significance of contaminant breakthrough time according to basic mathematical and physical models in geotechnical soil, and the calculation methods of contaminant breakthrough time and penetration depth are researched from the perspective of combining mathematical meaning and practical application needs. Moreover, the verified results provide insights into the prediction trends of contaminated groundwater. Finally, this method can provide a basis reference for the design, management and subsequent repair of contaminated groundwater in subsoils by considering different seepage velocities and anti-seepage layer characteristics.

II. MATERIALS AND METHODS

A. THE BASIC MODEL AND ITS SOLUTION

The mathematical model is a basic tool used to study the contaminant transport process and laws, and is an important theoretical foundation in the field of environmental geotechnical engineering [1, 2]. The hydrodynamic dispersion equation is the basic differential equation of contaminant migration in porous media [23-27], and the mathematical model consists of the basic differential equation, initial conditions and boundary conditions that describe the contaminant migration in actual problems [28].

The classic and widely used solute transport model is a continuous injection tracer model in a semi-infinite sand column without considering adsorption and decay, and the most basic model for contaminant migration is summarized in [28] as follows: ① A semi-infinite homogeneous medium column in the seepage zone. ② A one-dimensional groundwater flow in accordance with Darcy's law, and the seepage velocity of groundwater is a constant value. ③ The initial tracer concentration in the seepage zone is \( C(x,0)=0 \). ④ A constant concentration \( C=C_0 \) tracer is injected continuously at \( x=0 \) since \( t=0 \). The above generalized model can be showed in Figure 1.

![FIGURE 1. A generalized diagram of one-dimensional contaminant transport in uniform flow field.](image)

The above conceptual model is the basic mathematical model can be written as Equation (I) or Equations (1)–(4).

\[
\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} \quad (0 < x < +\infty, t > 0) \tag{1}
\]

\[
C(x,t) \bigg|_{x=0} = 0 \quad (x > 0) \tag{2}
\]

\[
C(x,t) \bigg|_{x=0} = C_0 \quad (t > 0) \tag{3}
\]

\[
C(x,t) \bigg|_{x=+\infty} = 0 \quad (0 \leq t) \tag{4}
\]

where \( C \) is the contaminant concentration (mg/L), \( D \) is the hydrodynamic dispersion coefficient (m\(^2\)/d) of contaminants in porous media, \( v \) is the groundwater seepage velocity (m/d), and \( x \) is the distance between the measuring point and the contamination source (m).

Using the Laplace variation, the analytical solution of the above model is

\[
C = \frac{C_0}{2} \text{erfc} \left( \frac{x-vt}{\sqrt{2Dt}} \right) + \frac{C_0}{2} \exp \left( \frac{xvt}{D} \right) \cdot \text{erfc} \left( \frac{x+vt}{\sqrt{2Dt}} \right) \tag{5}
\]
where \( \text{erfc}(u) \) is the residual error function and \( u \) is the function of \((x,t)\).

**B. MODEL UTILITY SIGNIFICANCE**

According to the basic assumptions of the convection-dispersion mathematical equation, the contaminant affects the entire computing domain once \( t=0 \) begins, and the theory is approximated to the thermal conduction model [29-31]. For Equation (5), the larger the calculated point distance from the boundary is, the smaller the error that occurs in the second item on the right[14, 18].

According to the mathematical law based on thermal conduction theory without considering the contribution of the second item on the right side, Equation (5) is rewritten as

$$\lambda = \frac{C}{C_0} = \frac{1}{2} \text{erfc}\left(\frac{x-vt}{2\sqrt{Dt}}\right)$$  \( (6) \)

Referring to the theoretical study of thermal penetration depth [31], it is considered that the contamination source at the origin has no practical effect in the area greater than \( x \), when the contamination source action time is less than breakthrough time \( t_j (t < t_j) \). Similarly, the penetration distance \( j \) of contaminant is the range of practical influence within the action time of the contamination source, and the impact is negligible when this range exceeds \( x \).

For the above considerations, the calculation standard of breakthrough time or penetration distance is the judgment standard of practical significance when using mathematical and physical methods. Thus, this clearly needs to be determined by the characteristics of the actual research subject or the field of expertise.

**C. MODEL COMPUTATIONAL ALGORITHM**

For the mathematical law of the thermal conduction equation, the region of \( 0-x \) is equivalent to the semi-infinite domain, and this is consistent with the mathematical laws reflected in the one-dimensional thermal conduction model. Thus, the computational problem of \( t_j \) can be studied using the semi-infinite domain model and its solutions.

For any breakthrough standard \( \lambda \), \( C(x, t_j) = \lambda C_0 \) and \( u \) is set as:

$$u = \frac{x-vt}{2\sqrt{Dt}}$$  \( (7) \)

According to Equations (6-7), \( \text{erfc}(u) = 2\lambda \), \( \text{erfc}(u) \) is a monotonically decreasing function that tends to zero rapidly with increasing \( u(x,t) \). The corresponding \( u \) can be verified by using the error function table after \( \lambda \) is determined. In addition, \( u \) monotonically decreases and \( \text{erfc}(u) \) monotonically increases with increasing \( t \); if the distance \( x \) lies between the measuring point and the source, the penetration velocity \( v \) and the dispersion coefficient \( D \) are known.

To obtain the breakthrough time with the penetrating depth, the relationship between \( u \) and \( t \) is studied by using the inverse method,

$$v^2t^2 - (2xv + 4u^2D)t + x^2 = 0 \quad \text{equation (8)}$$

$$t_j = \frac{xv + 2u^2D - \sqrt{(xv + 2u^2D)^2 - v^2x^2}}{v^2} \quad \text{equation (9)}$$

The above formula is the calculation formula of the breakthrough time \( t_j \) under the breakthrough standard \( \lambda \) (corresponding to \( \text{erfc}(u) = 2\lambda \)), and the value of \( t_j \) depends not only on the breakthrough standard \( \lambda \) but also on the flow field characteristics (the penetration rate \( v \), dispersion coefficient \( D \)) and the distance \( x \) between the measurement point and the source. It is worth noting that at this time, \( x, D, \) and \( u \) are known values, and \( v \) can be determined by the seepage field hydraulic slope and seepage coefficient of the actual problem according to Darcy’s law.

In actual sites, composite contamination is mostly used, and the transportation of contaminants in rock and soil bodies and groundwater bodies is quite slow, which is closely related to medium permeability and flow field conditions. Therefore, how to define the breakthrough time and establish a corresponding calculation method is worth further exploration. The simplified algorithm in this paper is more direct and simper than the current indirect algorithm, which needs to calculate the measuring point concentration repeatedly.

**III. RESULTS AND DISCUSSION**

**A. MODEL VERIFICATION**

For the model validation, three single-layer seepages of different thicknesses (1, 2 and 3 meters) were set for simulation calculation according to [19], and the results were compared with the finite element method and numerical method to show that the calculation results meet the actual requirements. For comparative analysis, the calculation method was recorded as UFM in this research, and SFM in the literature [19]. The permeability coefficient of the seepage layer was set to \( 1.0 \times 10^9 \text{ m/s} \), the breakthrough standard \( \lambda \) was set to 900, the effective diffusion coefficient was set to \( 2.5 \times 10^{10} \text{ m}^2/\text{s} \) and the block factor was set to 3.3. The calculated UFM results were compared with the SFM results in Figure 2.

Figure 2 shows that the breakthrough time of the impermeable layer decreased as the upstream head increased, regardless of which calculation method was employed. For example, when the upstream water head increased from 0.3 m to 10 m, the breakthrough time of the 2 m thick layer decreased from 27.5 to 7.2 years (decrease of 74%), while the algorithm breakthrough time of SFM decreased from approximately 25.0 to 7.0 years (decrease of 72%). With the decrease in the seepage layer thickness, when the thickness was reduced from 3 to 1 m at 0.3 m upstream of the water head, the breakthrough time was shortened from 54.0 to 7.9...
years (decrease of 85%), while the result of the SFM method decreased from approximately 49.0 to 7.0 years (decrease of 86%). The magnitude of the breakthrough time decline also increased with the upstream water head, and the greatest extent of reduction in breakthrough time was approximately 92.0% when the upstream water head was at 10 m.

**FIGURE 2.** Comparisons of UFM results for single impervious layer breakthrough time with SFM.

The breakthrough time of the single-layer anti-seepage layer calculated from this paper was basically consistent with that calculated by the existing research. The results indicated that the simplified calculation method can reliably estimate the breakthrough time of a single layer.

**B. PARAMETER RESPONSE REGULARITY**

Parameter response regularity was analyzed based on the analytical method and the numerical method for verifying the applicability of the analytical method. In this study, the mixed Euler-Lagrange method was used for solving convection-dispersion equation, which was widely used in different field problems [32, 33].

The response law of the model parameters was further studied using the algorithm for the breakthrough time proposed in this paper. The seepage speed was set to \( v = 0.0014 \) m/d, and the hydrodynamic dispersion coefficient was set to \( D_h = 4.9 \times 10^{-4} \) m\(^2\)/d. To cover most of the possible conditions, four impermeable layer thicknesses \( x \) (1.0, 2.0, 3.0, and 5.0 m) and different breakthrough standards \( \lambda \), which correspond to \( u \), were considered to calculate the different response laws of the model parameters. The above calculation results are showed in Figures 3–8.

From Figures 3–4, the thicker the impervious layer is or the greater the breakthrough standard is, the longer the breakthrough time becomes. Furthermore, the smaller the impermeable layer thickness is, the greater the relative error becomes between numerical solution and analytical solution. The maximum relative error is about 16% under the condition of \( x = 1 \) m.

For studying the variation of breakthrough time with different dispersion coefficients. The impervious layer thickness was set to \( x = 2 \) m, and dispersion coefficient was set to \( 0.5D_h, D_h, 2D_h \) and \( 5D_h \). The above calculation results are showed in Figures 5–6.

**FIGURE 3.** The analytical and numerical resolution of breakthrough times with different seepage thicknesses under different breakthrough criteria.

**FIGURE 4.** The relative error between analytical (\( t \)) and numerical (\( t' \)) resolution of breakthrough times with different seepage thicknesses.

From Figures 5–6, the smaller the dispersion coefficient is or the greater the breakthrough standard is, the longer the breakthrough time becomes. Furthermore, the greater the dispersion coefficient is, the greater the relative error becomes between numerical solution and analytical solution. The maximum relative error is about 25% under the condition of \( 5D_h \).

From Figures 7–8, the smaller the seepage speed is or the greater the breakthrough standard is, the longer the breakthrough time becomes. Furthermore, the smaller the seepage speed is, the greater the relative error becomes between numerical solution and analytical solution. The maximum relative error is about 16% under the condition of \( 0.5v \). In addition, the relative error is higher than other cases, this is because the second item on the right side is ignored of Equation (5).
According to the above calculation results from Figures 3–8, the $t_j$ is directly proportional to the $x$ and $\lambda$ and inversely proportional to the $v$ and $D_h$. From the relative error between numerical solution and analytical solution, the maximum relative error is about 25% under the condition of $5D_h$. That shows that the dispersion coefficient is more sensitivity on the analytical solution than other parameters. Moreover, the breakthrough time increases nonlinearly with the increase in the thickness of the anti-seepage material, or the decrease in the seepage velocity and the dispersion coefficient. The greater the breakthrough standard is, the longer the breakthrough time becomes.

**C. SENSITIVITY ANALYSIS**

The research on sensitivity analysis varies from different fields. It is an instrument for the assessment of the input parameters with respect to their impact on model output. Therefore, it is useful not only for model development, but also for model validation and reduction of uncertainty [34].

Up to now, there are many different methods of sensitivity analysis. In this research, modified Morris screening method was used, the sensitivity is expressed by a dimensionless index, which is calculated as the ratio between the relative change of model output and the relative change of a parameter. In order to improve the sensitivity discriminant parameters, an alternative approach to define the parameter variation is considered in which the parameters are not varied by a fixed percentage of the initial value but by a fixed percentage of the valid parameter range [35, 36].

The formula used to calculate sensitivity discriminant factor is as follows,

$$S = \frac{1}{n-1} \sum_{i=2}^{n-1} \left(\frac{Y_{i+1} - Y_i}{Y_a}\right) / P_a$$

(10)

Where $S$ is the discriminant coefficient of variable sensitivity, $Y_{i+1}$ and $Y_i$ are the model output calculated with the entered parameter value $P_{i+1}$ and $P_i$, respectively. $Y_a$ is the average value of $Y_{i+1}$ and $Y_i$, $P_a$ is the average value of $P_{i+1}$ and $P_i$, and $n$ is the running times of Morris model.
According to the $S$ value of the variable, the sensitivity of the parameters are ranked into four classes [36, 37], which are shown in Table 1. The greater the value is, the higher the sensitivity of the parameter.

| Class | Index | Sensitivity |
|-------|-------|-------------|
| I     | 0.00≤|S|<0.05 | Low         |
| II    | 0.05≤|S|<0.20 | Medium      |
| III   | 0.20≤|S|<1.00 | High        |
| IV    | |S|≥1.00 | Higher      |

According to the hydrogeological conditions in actual site, four parameters ($x$, $v$, $D_h$ and $\lambda$) are selected for the sensitivity analysis, and the initial values set for each parameter are shown in Table 2.

| Parameter | Value |
|-----------|-------|
| $x$ (m)  | 2     |
| $v$ (m/d)| 0.0014|
| $D_h$ (m$^2$/d) | 4.9×10$^{-4}$|
| $\lambda$ | 0.05 |
| $t_i$ (yr) | 1.53 |

Due to the actual site conditions, the parameters have a large variation range. The group of parameter values selected for sensitivity analyses are shown in Table 3.

| Parameter | Value |
|-----------|-------|
| $x$ (m)  | 0.5x |
| $v$ (m/d)| 0.2v |
| $D_h$ (m$^2$/d) | 0.5 |
| $\lambda$ | 1.0 |
| $t_i$ (yr) | 1.00 |

| Parameter | Value |
|-----------|-------|
| $x$ (m)  | 1.0x |
| $v$ (m/d)| 0.3v |
| $D_h$ (m$^2$/d) | 2.0 |
| $\lambda$ | 2.0 |
| $t_i$ (yr) | 1.53 |

| Parameter | Value |
|-----------|-------|
| $x$ (m)  | 1.5x |
| $v$ (m/d)| 1.0v |
| $D_h$ (m$^2$/d) | 3.0 |
| $\lambda$ | 2.5 |
| $t_i$ (yr) | 2.16 |

| Parameter | Value |
|-----------|-------|
| $x$ (m)  | 2.0x |
| $v$ (m/d)| 2.0v |
| $D_h$ (m$^2$/d) | 5.0 |
| $\lambda$ | 5.0 |
| $t_i$ (yr) | 2.54 |

| Parameter | Value |
|-----------|-------|
| $\lambda$ | 2.5x |
| $v$ (m/d)| 2.5x |
| $D_h$ (m$^2$/d) | 2.5x |
| $\lambda$ | 2.5x |
| $t_i$ (yr) | 5.34 |

| Parameter | Value |
|-----------|-------|
| $x$ (m)  | 0.5x |
| $v$ (m/d)| 0.2v |
| $D_h$ (m$^2$/d) | 0.5 |
| $\lambda$ | 1.0 |
| $t_i$ (yr) | 2.0 |

| Parameter | Value |
|-----------|-------|
| $x$ (m)  | 1.0x |
| $v$ (m/d)| 1.0v |
| $D_h$ (m$^2$/d) | 2.0 |
| $\lambda$ | 2.0 |
| $t_i$ (yr) | 2.5 |

| Parameter | Value |
|-----------|-------|
| $x$ (m)  | 1.5x |
| $v$ (m/d)| 1.5v |
| $D_h$ (m$^2$/d) | 3.0 |
| $\lambda$ | 3.0 |
| $t_i$ (yr) | 2.16 |

| Parameter | Value |
|-----------|-------|
| $x$ (m)  | 2.0x |
| $v$ (m/d)| 2.0v |
| $D_h$ (m$^2$/d) | 5.0 |
| $\lambda$ | 5.0 |
| $t_i$ (yr) | 2.54 |

Based on the sensitivity analyses performed for each group of parameter values, variations in the breakthrough time $t_i$ as the result of variations in the values of other parameters are shown in Figure 9. In addition, the relative sensitivities to changes in other parameters are shown in Table 4.

**TABLE 4. Relative sensitivity of $t_i$ to other parameters.**

| Parameter | $|S|$ | Grade |
|-----------|-------|-------|
| $x$       | 1.37  | IV    |
| $v$       | 0.46  | III   |
| $D_h$     | 0.55  | III   |
| $\lambda$ | 0.26  | III   |

Figure 9 shows that the $t_i$ is directly proportional to the $x$ and $\lambda$ and inversely proportional to the $v$ and $D_h$. The sensitivity of the $t_i$ to other parameters decreases as follows: $x > D_h > v > \lambda$. The sensitivity to $x$ is the highest, with a sensitivity grade of IV, and the sensitivity to $D_h$, $v$ and $\lambda$ are the same grade, with the sensitivity grade of III. That is, the sensitivity of the above four parameters is very high on $t_i$. The results show that the above four parameters need to be considered when the impervious layer are set. Moreover, this provide a theoretical basis for the design of impervious systems.

**IV. CONCLUSION**

According to the working on the convection-dispersion equation, the one-dimensional migration of the key contaminant indicator in the semi-infinite domain and its solution were investigated, taking into account the breakthrough standard, seepage velocity, and the anti-seepage material characteristics of dispersion and thickness.

(1) In different cases, the breakthrough time increases non-linearly with the increase in the thickness of the anti-seepage material, or the decrease in the seepage velocity and the dispersion coefficient. Furthermore, the greater the breakthrough standard is, the longer the breakthrough time becomes.

(2) Through comparative analysis of the analytical solution and the numerical solution, the results show that the calculation relative error is controllable and the calculation is feasible, that is, the approached algorithm of contaminant breakthrough time based on thermal penetration theory is feasible.
(3) Sensitivity analysis was carried out by using actual site data, and the sensitivity of the breakthrough time to each parameter decreases in the order $x > D_t > v > \lambda$. This shows that the above four parameters play important roles in the improving the breakthrough time of impervious system.

(4) The simplified formula for calculating the breakthrough time were proposed, the breakthrough standard should be set according to the characteristics of the actual research object or the expertise field.

(5) The breakthrough time is closely related to the breakthrough distance of contaminants; therefore, the relevant standards and calculation methods should be included in a unified research system. The proposed method is simpler and more convenient than the current model, and it can provide a reference for the design, management and subsequent remediation of contamination sites.

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