Design and Implementation of Numeric Solver for Simulation of Diffusion of Nuclide in Backfilled Material

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ABSTRACT

In this paper, a model for diffusion of nuclide in backfilled material is introduced, and discrete schemes presented, too. The algorithm to accomplish the simulation is given, to avoid error and exception that may occur during calculation, the check mesh algorithm is introduced. To implement a numeric solver for the simulation of diffusion of nuclide, several classes are designed, such as runtime class, mesh data class, environment class, calculation parameter class and calculation class. And then this solver is implemented with finite element method. Finally, the solver is used to calculate one case built for a 10000-years simulation of diffusion of nuclide in backfilled materials. The simulating result is satisfying, and the curve of nuclide concentration over time shows the nuclide concentration field becomes a stable one after about 3000 years.

Keywords: diffusion of nuclide; backfilled materials; discrete schemes; numeric solver; finite element method

1. INTRODUCTION

Nuclear wastes mean unwanted materials that contain unstable elements of alpha, beta and gamma radiation and produce heat meanwhile. Once those materials come into biosphere, water, air and soil will be polluted, and then enter the human body through a variety of means.

For example, one nuclear power station of 1000-megawatt produces wastes that may contain 10 kilograms of Np237 and 20 kilograms of Tc99 every year, it may take more than 1 million years to store those materials to meet the environmental challenge. So the methods of disposal of nuclear wastes impact the policy of one country’s nuclear power industry.

By 2012, there are 15 nuclear reactors in operation, and 26 reactors under construction in China, to handle all those wastes, Chinese government has decided to set up an underground research laboratory by 2020, and construct the underground nuclear waste repository by 2050 [1]. So the disposal of nuclear wastes is extremely urgent in China.

In general, nuclear wastes are stored in the geologic body underground about 500-1000 m, multi barriers are used to ensure the environmental safety, which includes engineered barriers, such as glass, canister, backfilled materials, and natural barriers such as host rock (granite, tuff, salt rock or clayrock).

Nowadays, lots of researches have been done on the diffusion of nuclide in backfilled materials [2-4] and host rock [5-7], Yu-jun Zhang has implemented 2-D and 3-D simulation of diffusion of nuclide [8-9].

The focus of this paper is the model of diffusion of nuclide in backfilled materials, design and implementation of numeric solver based on the model, finally, a case calculated by the solver is given to show the predicted distribution of nuclide concentration in backfilled materials within 10000 years.

2. GOVERNING EQUATIONS

Backfilled material is a kind of porous media, and the diffusion of nuclide in backfilled material is mainly affected by the temperature field and the porous media seepage field, in this paper, temperature field is treated as a stable one, and no impact of chemical reaction is involved, too. So the governing equation is listed as following[10].

\[
A \frac{\partial C}{\partial t} = \frac{\partial}{\partial x_l} \left( D_{ij} \frac{\partial C}{\partial x_l} \right) - V_j \frac{\partial C}{\partial x_i} - FC + Q
\]

where

- \( C \) : Nuclide concentration
- \( D_{ij} \) : Coefficient of hydrodynamic dispersion, equal to \( D_0 \cdot \alpha \beta \)
- \( D_0' = \alpha \sqrt{V} \)
- \( \alpha_r \) : Transverse and longitudinal dispersion coefficient
- \( V \) : Seepage field rate
- \( V_i \) : Seepage velocity in \( i \) th direction
- \( \Delta T \) : Difference between the current temperature and reference temperature.

F : Attenuation coefficient
Q : Internal source

\( D_0 \) is molecular diffusion coefficient and \( \eta \) is bending rate of Porous media. Furthermore, \( D_0 \) can be expressed as \( D_0 = \exp (\sigma \Delta T) \).

Among them \( D_0 \) is diffusion coefficient of molecules under a reference temperature, \( \sigma \) is a coefficient for correction and \( \Delta T \) is difference between the current temperature and reference temperature.

\( F \) is the attenuation coefficient
\( Q \) is the internal source
3. DISCRETE SCHEMES

Specifies a set of complete function sets \( w \), for each function \( w_k \):

\[
\int w_k \frac{\partial C}{\partial t} d\Omega - \int w_k \frac{\partial}{\partial x} (D_{ij} \frac{\partial C}{\partial x}) d\Omega + \int w_k \frac{\partial}{\partial y} (D_{ij} \frac{\partial C}{\partial y}) d\Omega + \int w_k FC d\Omega - \int w_k Q d\Omega = 0
\]

With the division integral formula:

\[
\int w_i \frac{\partial}{\partial x} (D_{ij} \frac{\partial C}{\partial x}) d\Omega = -\int \frac{\partial w_i}{\partial x} (D_{ij} \frac{\partial C}{\partial x}) d\Omega + \int w_i D_{ij} \frac{\partial C}{\partial x} d\Omega
\]

We can obtain form equation (3):

\[
\int w_i A \frac{\partial C}{\partial t} d\Omega + \int \frac{\partial w_i}{\partial x} D_{ij} \frac{\partial C}{\partial x} d\Omega + \int w_i V \frac{\partial C}{\partial x} d\Omega + \int w_i FC d\Omega = \int w_i Q d\Omega
\]

Here \( \bar{q} = D_{ij} \frac{\partial C}{\partial x} n \) represents flux of concentration on the boundary.

Discretize concentration \( C \) into a linear superposition of a group of shape functions (For its own node, the value is 1 while for the other nodes the value is 0) as \( C = \sum_n a(t) w_n \) (\( m \) represent each discrete points).

We also specifies \( w_k = N_k \)

Finally we obtain:

\[
A \int N_i \frac{\partial C}{\partial t} d\Omega + \int \nabla \cdot [N_i \eta [D] \nabla (\sum_m a(t) w_m)] d\Omega + \int N_i (\nabla \cdot \nabla (\sum_m a(t) w_m)) d\Omega + \int N_i \sum_m a(t) w_m d\Omega = \int N_i \bar{q} d\Omega + \int N_i Q d\Omega
\]

Define \( a^T = \{a_1, a_2, a_3, ..., a_m\}^T \), equation (5) can be expressed into matrix form:

\[
G \frac{da}{dt} + Ka^T = f
\]

In equation (6):

\( G \) is a \([m \times m]\) matrix, \( G_{km} = A \int N_k N_m d\Omega \)

\( f \) is a \([m \times 1]\) vector, \( f = f_1 + f_2 \),

\( f_1 = \int Q N d\Omega \) and \( f_2 = \int \bar{q} N d\Omega \)

\( K \) is a \([m \times m]\) matrix, \( K = K_1 + K_2 + K_3 \)

Equation (6) is a group of linear differential equations that can be solved numerically by finite difference method.

4. ALGORITHM

To implement the numeric solver, before solve the matrix, 3 matrixes must be loaded, such as stiffness matrix (K matrix), factor load matrix (F matrix) and time evolution matrix (C matrix). The process of matrix loading is determined by mesh data and boundary conditions, so the algorithm can be expressed in figure 1.
Because some control points may exist in the mesh data, which means those points are listed in mesh point data, but never appear in tetrahedron data. To avoid the error and exception that may happen during solving process, before loading matrix, mesh data must be checked if those points exist. The check process flow is shown in figure 2.

5. DESIGN OF CLASSES
Several classes are designed to construct the numeric solver, such as runtime class, environment class, calculation class, mesh data class and calculation parameter class. It’s good to design solver with class, the reasons may be independence, encapsulation and easy to maintain the software. The purposes of different classes are shown in table 1.

<table>
<thead>
<tr>
<th>Class</th>
<th>Purpose</th>
</tr>
</thead>
<tbody>
<tr>
<td>Run Time</td>
<td>Read and store case runtime information, such as start Time, end Time, Case folder, Time interval for calculation and Time interval to write data file. That information can be accessed anytime while calculating.</td>
</tr>
<tr>
<td>Environment</td>
<td>Read and store case information, especially mesh data file’s full path and case files. This class checks whether those files exists indeed to ensure Mesh data class can read the proper files</td>
</tr>
<tr>
<td>Mesh Data</td>
<td>Read mesh data files and boundary condition file, and store those data into inner vectors respectively. Mesh data contain mesh point, face triangle, tetrahedron and boundary conditions and can be accessed anytime while calculating.</td>
</tr>
<tr>
<td>Calculation parameter</td>
<td>Read and store calculation parameters, such as internal source, attenuation coefficient, etc. Those parameters can be accessed anytime while calculating.</td>
</tr>
<tr>
<td>Calculation</td>
<td>Read mesh data from mesh data class, read runtime information from Run Time class, and produce K, F, C matrixes, then solve the equation and get the solution vector.</td>
</tr>
</tbody>
</table>
Because the calculation class needs access mesh data from mesh data class directly, so the calculation is designed as a friend class of mesh data class. The connections among classes are shown in figure 3.

6. SIMULATION OF DIFFUSION OF NUCLIDE IN BACKFILLED MATERIALS

Based on the model of diffusion of nuclide in porous media and the design of classes, a numeric solver can be implemented. The solver can be run to validate the model or to predict the long-term distribution of nuclide in backfilled materials. Because nuclide may decay, it’s better to simulate long-term distribution of nuclide with attenuation coefficient.

Here is one long-term simulation of diffusion of nuclide with attenuation coefficient as shown in figure 4.

(a) Distribution of nuclide
We can see that after about 3000 years of diffusion, the nuclide concentration field comes to be stable, and on more changes of concentration occur. It’s assumed that the host rock doesn’t allow the migration of nuclide, and temperature doesn’t affect the host rock, too, so the nuclide concentration of point on the outer wall stays unchanged after reaching stable.

In this simulation, it’s assumed the diffusion is isotropic, so the distribution of nuclide is also isotropic, but indeed, the diffusion can be set anisotropic according to the actual demands.

7. CONCLUSIONS

In this paper, a numeric solver is designed and implemented based on the nuclide diffusion model. Backfilled material is a kind of porous media indeed, so this model is set up based on Darcy’s law. Several classes are designed to implement the solver, and each class has its unique purpose. The solver needs mesh points’ data, mesh face triangles’ data, mesh tetrahedrons’ data and initial boundary conditions, because the size of mesh varies every time, several vectors are used to store mesh data, and several 2-dimensioned matrices are used to store private data and calculate. After the mesh and initial conditions are given, we can use the solver to calculate and simulate long-term distribution of nuclide in backfilled materials. The simulating results should be an assessment for disposal of nuclear wastes.

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REFERENCES


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