MDPSA code verification for advective-dispersive mass transport in Porous Media

Ji-Woong Han, Yong-Soo Hwang and Chul-Hyung Kang
Korea Atomic Energy Research Institute, #150, DeokjinDong, YuseongGu, Daejeon, Korea, jwhan@kaeri.re.kr

1. Introduction

As a part of the mid- and long-term nuclear research and development program in Korea[1], KAERI is developing a new probability safety assessment program. A newly developed program(MDPSA code) is designed to be capable of probabilistic assessment of radionuclide in multi-dimensional regions both of a fracture network and of a porous medium such as a top soil and buffer and backfill layers. Before we apply it to a real problem, the accuracy of the solution should be validated. In order to determine the accuracy of the numerical results, comparison with an exact solution is often utilized. In the comparing method, a simple geometry with a known, relatively simple analytic solution is used for comparison with the numerical code.

In order to verify the MDPSA code performance in porous medium geometry, a series of calculations for mass transport have been done and presented in this study. A porous medium geometry with a known, relatively simple analytic solution is used. Advection and diffusion transport phenomena were examined. Dead-end pore effect[5] in porous medium, which can cause long delays in the travel time, was simulated with rock matrix diffusion equation in fractured medium model. Finally overall mass transport performance for a porous medium was verified in a simple geometry.

Based on the calculation results that were in good agreement with analytic solutions, it can be said that the numerical results of MDPSA code are physically reliable for prediction of mass transport in porous medium.

2. Methods and Results

This program is developed on the basis of finite volume method assuming steady-state, constant density groundwater flow and the related numerical scheme can be found in the preceding references[2-5]. A series of calculation for verifying the program is as follows ;

2.1 Advection and Diffusion

This case consists of advection and diffusion in a domain $0 \le x \le L$ with the initial condition that the concentration is zero throughout the domain and the radionuclide boundary conditions such as $C = 1 \;\; at \;\; x = 0$, $C = 0 \;\; at \;\; x = L$. The grid blocks were all taken to have sides of length 1. q_x was taken to be 1 and the other components of the flow were taken to be zero. Retardations, porosity, diffusion coefficient were taken to be 1 respectively. The boundary conditions were taken to be zero flux on the boundaries of the model normal to the y and z axes. In Table 1, a comparison of the results obtained from the analytic solution for the discretised equations is presented. As can be seen the agreement is very good.

Table 1 Comparison of analytic and numerical solutions

x	Analytic Solutions	Numerical Solutions
0	1.000000	1.0000
1	0.585714	0.5857
2	0.342857	0.3429
3	0.200000	0.2000
4	0.114286	0.1143
5	0.057143	0.0571
6	0.000000	0.0000

2.2 Retardation

In a porous medium there could be many dead-end pores, in which the solute is trapped and from which it can escape only by molecular diffusion. In this study rock matrix diffusion equation in fractured medium model was utilized for the simulation of this phenomenon in porous medium. This can be modeled as the case consists of pure diffusion with the concentration initially 1 and with the distance available for diffusion into the rock matrix taken to be unlimited. This has an analytic solution as follows;

$$C = e^{\frac{4D_{\text{int}}t}{a^2}} erfc\left(\frac{2\sqrt{D_{\text{int}}t}}{a}\right) \tag{1}$$

Where D_{int} is the intrinsic diffusion coefficient and a the aperture of fracture. Corresponding calculations were also undertaken with MDPSA code. In order to include the effect of dead-end pore, a simple model is adopted, which represents one-dimensional diffusion into the rock matrix between equally spaced parallel fractures. This effect can be adopted by adding the following term to radionuclide transport equation.

$$\frac{2D_{\text{int},\alpha}\phi_\alpha}{a}\frac{\partial C'_\alpha}{\partial w}\bigg|_{w=0} \tag{2}$$

where C'_α is the concentration of the radionuclide in the rock matrix, w is the distance from the fracture and

ϕ_α is the porosity. C'_α is determined by the following transport equation

$$\alpha_\alpha \frac{\partial C'_\alpha}{\partial t} = D_{\text{int},\alpha} \frac{\partial^2 C'_\alpha}{\partial w^2} \quad (3)$$

together with boundary conditions

$$C'_\alpha = C_\alpha \quad at \quad w = 0 \quad (4)$$

$$D_{\text{int},\alpha} \frac{\partial C'_\alpha}{\partial w} = 0 \quad at \quad w = d \quad (5)$$

Where α_α is the capacity factor for the radionuclide and d is the maximum distance available for diffusion into the rock matrix. A 7X5x3 grid was used. The time step size was taken to be 10^4. The grid blocks were all taken to have sides of length 1. The flow was taken to be zero. The retardation was taken to be 1. The accessible flowing porosity was taken to be 0.01 and the intrinsic diffusion coefficient was taken to be 10^{-11}. The boundary conditions were taken to be zero flux on the all the boundaries of the model. From Figure 2 we can recognize that two lines are overlapped closely.

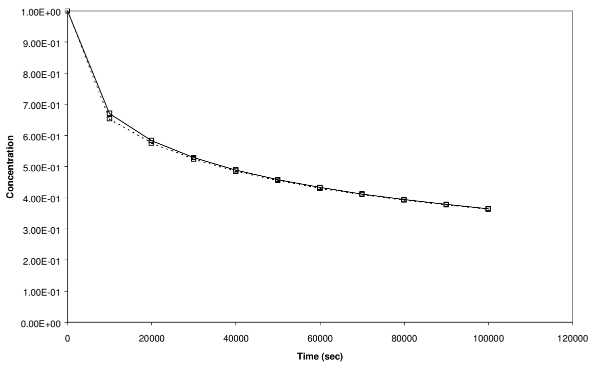

Figure 2. Comparison of analytic and numerical solutions with time

2.3 Advection, Dispersion and Retardation

Finally one dimensional geometry was selected that consists of advection, dispersion and retardation. The concentration in the domain was taken to be zero initially. The boundary conditions are that the concentration is 1 at the inlet end of the domain and 0 at the outlet end. The values of each parameter for this case are listed on Table 2. An analytic solution to this case was obtained using Laplace transforms, which were inverted numerically using the Talbot algorithm[6].

Table 2 Allocated values for each parameter

Parameter	Value
Length of Domain	1E+4
Head drop across the domain	50
Porewater diffusion coefficient	1E-9
Rock permeability	1E-11
Flowing porosity	1E-2
Longitudinal dispersion length	50
Retardation	1
Intrinsic diffusion coefficient	5E-11

A 100x1x1 grid was used with the grid block sides taken to be 100 in each direction. The boundary conditions were taken to be zero flux on the boundaries of the model normal to y and z axes.

In Figure 3, a comparison of the solution obtained by numerical inversion of the Laplace transform with the results obtained using MDPSA program is presented. It shows a good agreement between two solutions.

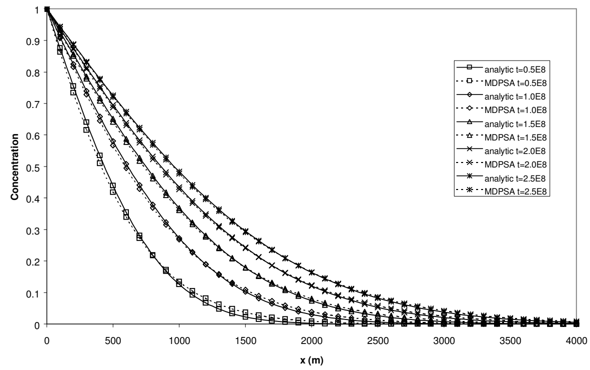

Figure 3. Distribution of radionuclide concentration

3. Conclusion

In this study a series of fundamental calculations and comparison processes with analytic solution have been done for the verification of MDPSA program in porous medium geometry. Every numerical solution shows a good agreement with analytic one. From these results MDPSA program can be said to predict mass transport phenomenon in porous medium reasonably well.

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