A NOVEL APPROACH FOR RADIONUCLIDE TRANSPORT IN INHOMOGENEOUS CRYSTALLINE ROCKS USING WAVELET GALERKIN METHOD

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Abstract: - This work develops efficient algorithms for numerically solving the nuclide migration through geosphere of performance assessment for the high level radioactive waste (HLW) using Wavelet Galerkin Method (WGM). From mathematical point of view the problem of convection diffusion type but the parameters are highly varying. Another particularity is the very concentrated nature of the spatio-temporal source.
The model which is a very coarsely wavelet-based discretization model, devised to be very fast due to the compactly support nature of the Daubechies' wavelet. We tested our WGM algorithms with different cases include single isotope calculations and decay chain calculations. The results show that WGM calculations are very accurate compared to other conventional methods.

Keywords: Wavelets, geological disposal, connection coefficients, compactly supported, crystalline rock

1. Introduction

The host rock under consideration is crystalline overlaid by a series of sedimentary rocks [1]. In-site investigations show that the crystalline is inhomogeneous and water-conducting zones can be found. Water flow can take place in the fractures embedded in these zones. Flow does not occur uniformly in the fractures, but rather is concentrated in channels that arise, from variation in aperture and the presence of infill material. There are many potential transport paths through the host rock, each comprised of one or a series of channels. The variability in the length, transmissivity and other transport-relevant properties of the transport paths, as well as interconnections between paths, gives rise to mechanical dispersion. Transport along these paths is retarded by diffusion into segment water in the pores of the rock matrix surrounding the channels and by sorption on infill and rock matrix pores.
This problem is of convection diffusion type with highly varying parameters from one medium to other. Another particularity is the very concentrated nature of the spatio-temporal source. The complexity of this situation makes it difficult to obtain analytical solution for the radionuclides transport. Standard numerical methods require a detailed discretization. Therefore, nuclide transport calculations would be very time consuming if they were made using standard numerical methods. To circumvent these problems, a technique has been developed that uses the advantages of the compactly supported wavelet. Compactly supported wavelets have recently been applied to the numerical solution of ordinary and partial differential equations with encourage results [2,3]. The most frequently used technique is the

Wavelet Galerkin Method (WGM) [4]. It has shown to be powerful tool especially for the non-linear differential operators due to the fact that it possesses several useful properties such as orthogonality and compactly support [5].

This work presents a useful tool to calculate the transport of the radionuclides in the geospheric, accounting for all possible paths by which the nuclides are transported to the faults and subsequently to the biosphere. An attempt to verify the model is made. Calculating the nuclide transport for simple test cases carries out this verification. The comparison is carried using analytical or accurate numerical code.

2. Problem Formulation

2.1 Daubechies' Wavelet

Among many wavelets can be used as a complete coordinate function, the Daubechies' wavelet has been chosen because it is defined a class of compactly supported wavelet. Briefly, let $\phi(x)$ be a solution of the scaling relation:

$$\phi(x) = \sum_{k=0}^{N-1} a_k \phi(2x-k) \tag{1}$$

where $\phi(x)$ is the scaling function. The associated wavelet function $\psi(x)$ is:

$$\psi(x) = \sum_{k=-N}^{1} (-1)^k a_{1-k} \phi(2x-k) \tag{2}$$

Where N is the wavelet order and it is positive even integer, and a_k is the collection of coefficients that satisfy the following conditions. From the normalization of the scaling function $\int \phi(x)dx = 1$, the first condition can be written as:

$$\sum_{k=0}^{N-1} a_k = 2 \tag{3}$$

The translations of $\phi(x)$ are required to be orthonormal,

$$\int \phi(x-k)\phi(x-m)dx = \delta_{k,m} \tag{4}$$

This formula implies the second condition:

$$\sum_{k=0}^{N-1} a_k a_{k-2m} = \delta_{0,m} \tag{5}$$

In all the formulas above δ represents the Kronecker delta function. Smooth wavelet function requires the moment of the wavelet to be zero,

$$\int x^m \psi(x)dx = 0 \tag{6}$$

Formula (6) implies the third condition:

$$\sum_{k=0}^{N-1} (-1)^k k^m a_k = 0, (m = 1, ..., N/2-1) \tag{7}$$

For the coefficients are satisfying with the above conditions, the functions, which consist of translations and dilations of the scaling function ($\psi(2^j x-k)$), form a complete and orthonormal basis. The relation between two functions is expressed as:

$$V_j = V_{j-1} \oplus W_{j-1} \tag{8}$$

where $\oplus$ denotes the orthonormal sum, and

$$V_j = 2^{j/2} \phi(2^j x-k) \tag{9.a}$$

$$W_j = 2^{j/2} \psi(2^j x-k), \tag{9.b}$$

for the integer k. And j is the dilation parameter, which is used as a scale. In the approximation of the differential equation, j is also the approximation level. For a certain value of j and N, the support of the scaling function $\phi(2^j x-k)$ is given as follows:

$$\sup(\phi(2^j x-k)) = \left[\frac{k}{2^j}, \frac{N+k-1}{2^j}\right] \tag{10}$$

As the scaling function yields a complete coordinate function basis, it can be used to expand general function as follows:

$$f(x) = \sum_k 2^j c_k \phi(2^j x-k) \tag{11}$$

Here it is worth emphasizing that there are two-convergence properties, used in the expansion (11). One is the uniform convergence for the level of approximation in relation to the dilation order j, and the other is the rapid convergence for smoother scaling function, which relates to the wavelet order N. These properties are not shared at the same time by the conventional classical orthogonal functions. The balance between N and j plays very important role for getting an accurate solution in an adequate time.

2.2 Governing Equations

The transport paths are modeled as parallel walled openings in which transport occurs by advection and dispersion and at a given time, nuclide concentration varies only in the flow direction. Figure 1., shows transport processes in a path comprising a single channel within a fracture, advection and dispersion are modeled in one spatial dimension only in the flow direction. Matrix diffusion is also modeled in one

spatial dimension normal to the plane of the fracture. In reality, fractures and channels can vary widely in their properties. In order to take into account the heterogeneity of real fractures and channels with respect to transmissivity, the present work considers transport along set of representative channels, each assigned different transmissivity. The multi-pathway model represents a step toward realism. In order to set the transmissivity of the model pathways, a probability distribution function (pdf) for the transmissivities in the host rock is descretized into 48 segments, with the channels in each segment being represented by a single, representative model pathway [1].

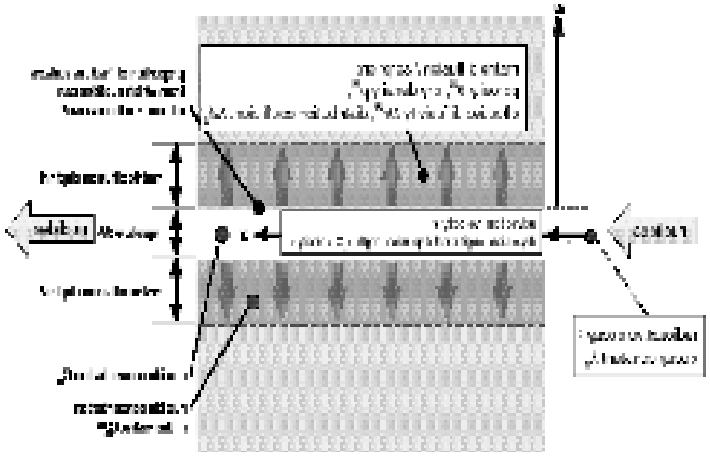

Fig.1. Illustration of the processes considered in the parallel plate model.

Based on the above model, the weighted nuclide release rate from the EBS to the model pathways $f_n(T_i,t)$, is defined as:

$$f_n(T_i,t) = P(T_i).f_n^{buffer \to hostrock}(t) \qquad (12)$$

where T_i is the median value of the transmissivity in segment i m^2s^{-1}, $P(T_i)$ is the probability of segment i, which is assigned according to the probability that the transmissivity of a randomly sampled channel in the host rock lies in the range of transmissivity in the segment i, $f_n^{buffer \to hostrock}(t)$ is the nuclide release rate per vitrified waste package $mol/\sec$ calculated from the EBS model [6], n is the nuclide ID, and t is the time. The governing equations expressing nuclide transport in one-dimensional parallel-plate fractures and in the matrix under steady state groundwater flow conditions are as follows:

$$R_n^f \frac{\partial C_n^f}{\partial t} = \frac{\partial}{\partial x} D_L \frac{\partial C_n^f}{\partial x} - \nu \frac{\partial C_n^f}{\partial x} - R_n^f \lambda_n C_n^f + R_{n-1}^f \lambda_{n-1} C_{n-1}^f + \frac{F}{b} D_e^m \frac{\partial C_n^m}{\partial \omega}\bigg|_{\omega=0} \qquad (13)$$

$$R_n^m \frac{\partial C_n^m}{\partial t} = \frac{\partial}{\partial \omega} D^m \frac{\partial C_n^m}{\partial \omega} - R_n^m \lambda_n C_n^m + R_{n-1}^m \lambda_{n-1} C_{n-1}^m \qquad (14)$$

Where, b half of the fracture aperture m, ν flow velocity in the fractures $m/\sec$, D_L dispersion coefficient in the fractures $m^2/\sec$ $(=\alpha_L \nu + D_0)$, α_L longitudinal dispersion length m, D_0 diffusion coefficient in free water $m^2/\sec$, λ_n decay constant $\sec^{-1}$, F proportion of fracture surface from which nuclides can diffuse into the matrix, D_e^m effective diffusion coefficient $m^2/\sec(=\theta^m D^m)$, θ^m matrix porosity, D^m diffusion coefficient in the matrix pores $m^2/\sec$, C_n^f, C_n^m nuclide concentrations in the fracture and in the matrix mol/m^3, x transport distance m, ω perpendicular distance into the matrix from the fracture surface m, and t the time. The suffices n, f and m are represented a nuclide, fracture and matrix respectively. In addition, R_n and R_n^m represent the retardation coefficients for nuclide n in fracture and in the matrix respectively, and are expressed by the following formulas with the assumption of linear, reversible and instantaneous sorption:

$$R_n = 1 + \frac{Ka_n}{b}, \quad R_n^m = 1 + \frac{\rho^m Kd_n^m}{\theta^m} \qquad (15)$$

where, Ka_n is the distribution coefficient for the fracture surface m, Kd_n^m is the distribution coefficient for the rock minerals in the matrix m^3/kg and ρ^m is the dry density of the matrix kg/m^3.

The initial concentration in the fracture and matrix assumed to be zero

$$C_n^f(x,0) = C_n^m(x,\omega,0) = 0 \qquad (16)$$

The weighted nuclide release from the EBS is taken as the boundary condition for the nuclide transport in the model pathway with tramsmissivity T_i,

$$A_f\left[\nu C_n^f - D_L \frac{\partial C_n^f}{\partial x}\right]_{x=0} = f_n(T_i,t) \qquad (17)$$

where A_f is the fracture cross section (= aperture x fracture unit width) m^2. The boundary condition at the fracture surface and at the maximum depth for matrix diffusion, d m, are expressed as follows:

$$C_n^f(x,t) = C_n^m(x,0,t) \qquad (\omega = 0) \qquad (18)$$

$$\frac{\partial C_n^m}{\partial \omega} = 0 \qquad (\omega = d) \qquad (19)$$

The nuclide release rate from the host rock per vitrified waste package is calculated from:

$$g_n(t) = \sum_{i=1}^{J} h_n(T_i,t) \qquad (20)$$

where, $h_n(T_i,t)$ is the nuclide release rate from the model pathway with transmissivity T_i, T_i is the median value of the transmissivity in segment i m^2s^{-1}, and J is the total number of the segment.

Due to the boundary condition (16), which couples the functions $C_n^f(x,t)$ with $C_n^m(x,\omega,t)$, the problem is two-dimensional in space in the sense that equation (13) has to be solved for every x-value. Let us consider the function $c(x,\omega)$ defined in a closed rectangle domain, then it can be approximated as

$$c(x,\omega) = \sum_{k=0}^{N-1}\sum_{l=0}^{N-1} c_{k,l}\, 2^p \phi(2^j x - k)\phi(2^j \omega - l) \qquad (21)$$

Let $C_{k,l} = 2^j c_{k,l}$, $X = 2^j x$, and $W = 2^j \omega$, and substitute equation (21) into equations (13), and (14), and take the inner products with $\phi(X-p)\phi(W-m)$, we get

$$\frac{dC_n^f}{dt} = D_L \sum_{k,l=0}^{N-1} (C_n)_{k,l}\Omega_{k,p}^{2,0}\delta_{l,m} - \nu \sum_{k,l=0}^{N-1} (C_n)_{k,l}\Omega_{k,p}^{1,0}\delta_{l,m}$$
$$- \lambda_n \sum_{k,l=0}^{N-1} (C_n)_{k,l}\delta_{k,p}\delta_{l,m} + \lambda_{n-1} \sum_{k,l=0}^{N-1} (C_{n-1})_{k,l}\delta_{k,p}\delta_{l,m}$$
$$+ \frac{F}{b} D_e^m \sum_{k,l=0}^{N-1} (C_n)_{k,l}\Omega_{l,m}^{1,0}\Big|_{\omega=0} \qquad (21)$$

$$\frac{dC_n^m}{dt} = \frac{D^m}{R_n^m} \sum_{k,l=0}^{N-1} (C_n)_{k,l}\Omega_{l,m}^{2,0} - \lambda_n \sum_{k,l=0}^{N-1} (C_n)_{k,l}\delta_{k,p}\delta_{l,m}$$
$$+ \frac{R_{n-1}^m}{R_n^m}\lambda_{n-1} \sum_{k,l=0}^{N-1} (C_{n-1})_{k,l}\delta_{k,p}\delta_{l,m} \qquad (22)$$

Where Ω it the connection coefficient on unbounded domain as defined by the expression

$$\Omega_{l_1,l_2}^{d_1,d_2} = \int_{-\infty}^{\infty} \phi^{d_1}(x-l_1)\phi^{d_2}(x-l_2)dx \qquad (23)$$

The superscripts d_1 and d_2 refer to the differentiation. The most expedient strategy available for the evaluation of these connection coefficients is given in [7]. The connection coefficients should be precomputed. The resulting tables are then read in the time marching procedure. Using this approximation and defining according to the mesh numbering shown in Fig. 2:

$$c(x_1,t) = f_1,\ c(x_2,t) = f_{J+1},\ldots\ c(x_I,t) = f_{(I-1).J+1}$$
$$c(\omega_2,t)\big|_{x=x_1} = f_2,\ ,\ldots\ldots\ldots\ldots\ c(\omega_J,t)\big|_{x=x_1} = f_J$$
$$c(\omega_2,t)\big|_{x=x_I} = f_{(I-1).J+2},\ \ldots\ldots\quad c(\omega_J,t)\big|_{x=x_I} = f_{I.J}$$

Following the approach of using wavelet Galerkin discretization approach, we obtain a system of nonlinear ordinary differential equations of the form:

$$\frac{dF_i(t)}{dt} = \sum_{h=1}^{I.J} V_{ih} F_h(t) \qquad (24)$$

In order for the algorithm to resolve all the structures, the basis of active wavelet and, consequently the computational grid should be adapted dynamically in the time to reflect local changes in the solution. The system is solved using the fifth-order gear implicit integration algorithm [9].

3. Problem Solution

Verification is addressed by comparing the results given by the model with analytical solutions and by comparison with a verified numerical code. The accuracy of the solution is investigated by defining test cases.

In the first test case, the values of the source term $f_n(T_i,t)$ in the repository is read from a separated data file obtained from the calculation of radionuclide migration in the engineered barrier system [6]. The analytical solution can be obtained by simplify the

problem to such an extent that simple solution emerge. Neglecting the dispersion in the fracture, $D_L = 0$, take an infinite medium, a simple upstream boundary condition, $C_0(t) = C_0 e^{-\lambda t}$, and consider a single decaying species only. Furthermore, we assume that the width of altered zone (and the fractures' distance) is very large and the fracture half-width very small compared to the penetration depth into the matrix. The solution in the fracture is given by

$$C(x,t) = C_0 e^{-\lambda t} erfc\sqrt{\frac{\tau_0}{t}}\ ,\ \tau_0 = \left(\frac{x}{2b}\frac{\varepsilon}{\nu}\right) R_n^m D_m$$

Results obtaining for the test case are shown in Fig.3 for various wavelet-dilation orders pair. At long time a good accuracy is obtained regardless of the wavelet discretization. The choice of wavelet-dilation order is only important at the early time. Better accuracy is obtained by increasing the wavelet-dilation order pair.

In the second test case, a transport of Np-237 is calculated as a single species. The obtained normalized flux using WGM is compared with the RANCHMD codes, a well verified computer program, as shown in Fig. 4. The comparison shows that, WGM with wavelet order of 10 and dilation order of 6 is accurate compared to the RANCHMD [8] code with relatively small discretization steps. The running time requires for WGM is less than that required for RANCHMD. Using higher dilation order increases the accuracy of the WGM. RANCHMD uses a very detailed discretization and high Lagrange interpolation order to achieve such accuracy. WGM approach is requiring less memory size than the one requires for RANCHMD.

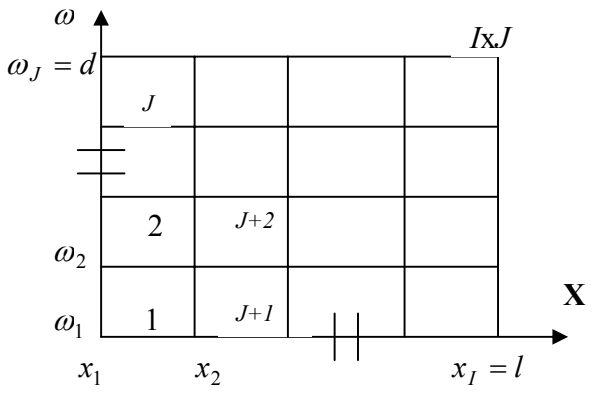

Fig. 2. Mesh Space System

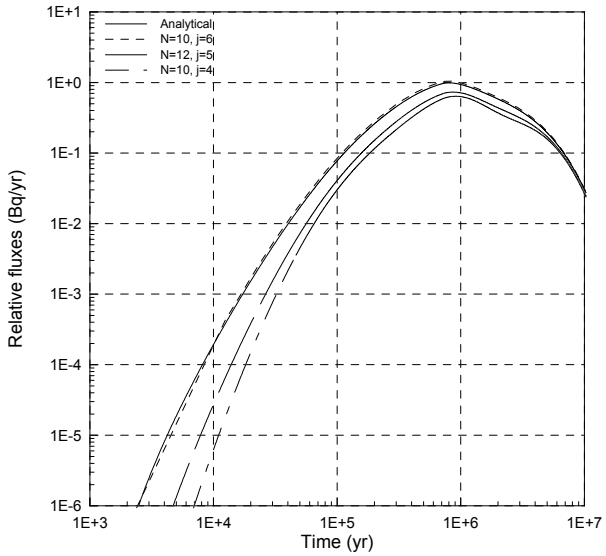

Fig.3 Relative fluxes for different wavelet-dilation orders pair and their comparison to analytical solution.

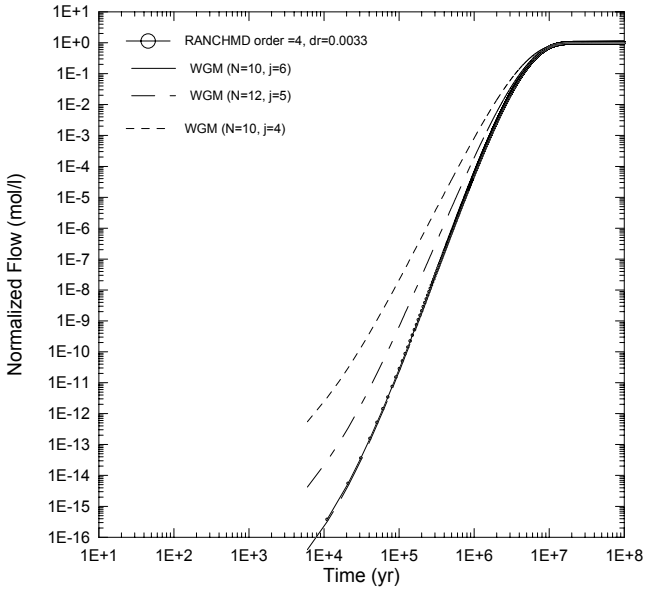

Fig.4 Relative fluxes for different wavelet-dilation orders pair and their comparison to RANCHMD code.

4. Conclusion

The approach of using wavelet theory is a useful tool to model the transport of single nuclides or

radionuclides chains in the far field of a repository. The model, which is coarsely discretized wavelet Galerkin, is devised to be very fast and efficient proper selection of the wavelet order and dilation order at sensitive points such as the interface between the fracture and the matrix, and at the entrance of the fracture where other models require detailed discretization. In general, the verification analysis showed that the accuracy of wavelet based model is good when it compared with models that use a very detailed discretization. The accuracy is sufficient in many cases for wavelet order of 10, which insure the smoothness and dilation order of 6, which gives finer solution at the fracture matrix interfaces considering that uncertainties in the parameter values, such as the transmissivity and distribution coefficient, are considerably more significant.

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