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Verification of a fracture network transport model including two-dimensional rock matrix diffusion

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Abstract The movement of radionuclides in saturated fractured rock, from the near field of a radioactive waste repository to the biosphere, is modelled as a part of a model chain in repository performance assessment. In order to use the potential of the geosphere as a barrier to radionuclide migration, the geosphere transport code PICNIC has been developed to take account of both small-scale and large-scale flow path heterogeneities. To ensure the reliability of such a code the verification described here is essential. PICNIC is verified to deal with transport of single nuclides and nuclide decay chains in a network of fractures with adjacent heterogeneous rock matrix for one-dimensional or two-dimensional matrix diffusion. Therefore analytical results are used, code cross-comparisons and discretization tests are performed. As an example, the verification of two-dimensional matrix diffusion into a homogeneous rock block is considered. The capability to deal reliably with two-dimensional matrix diffusion is novel in fracture network modelling.

INTRODUCTION

In the context of safety assessment of radioactive waste repositories, complex radionuclide transport models play a major role. In recent Swiss safety assessments, such as Kristallin-I (Nagra, 1994) for the Swiss high-level radioactive waste disposal concept, a model chain for the near field, the far field, and the biosphere has been used. However, an important drawback in Kristallin-I was the limitation in modelling capability to account for the geosphere heterogeneity. In strong contrast to this limitation, great effort has been put into investigating the heterogeneity of the geosphere as it impacts on the hydrology, defining the large-scale heterogeneity of the geosphere (Nagra, 1994; Thury *et al.*, 1994). Structural geological methods have been used to look at the geometry of the flow paths on a small scale. To efficiently make use of the knowledge of the heterogeneity of the geosphere, the PICNIC project has been established as a cooperation of PSI/Nagra and QuantiSci, to provide a new geosphere transport model for Swiss safety assessment of radioactive waste repositories. PICNIC can deal with all processes considered in the geosphere model RANCHMD (Hadermann & Rösel, 1985) generally used in the Kristallin-I study, and in addition explicitly accounts for the heterogeneity of the geosphere on two spatial scales, cf. Table 1. To ensure the reliability of such a code, the verification described here is of

Table 1 The application range of PICNIC is the combination of the points A–F described in the second column. The base case includes advective and dispersive transport in a single leg in the area of flowing water, together with linear sorption in the area of flowing water and in the rock matrix. The "code levels" correspond to the PICNIC flow scheme (Table 2).

	Features	Code levels involved
A	Single nuclides or nuclide decay chains	All
B	A single leg, a pathway (legs in series), or a network of legs	6, 7 for pathways and networks
C	Three different leg outlet boundary conditions	4
D	Different shapes of the source; one or more sources	5, 9, 10
E	1D-MD, 2D-MD, different rock matrix geometries	1
F	Together with the variation of all parameters	All

primary importance. This paper gives the structure and an overview of the verification of the PICNIC code. Moreover it presents—to our knowledge—for the first time, reliable calculations with two-dimensional matrix diffusion (2D-MD) relevant to geosphere transport modelling. This is possible because of a recent further development of the PICNIC code.

FLOW SCHEME AND POSSIBLE ERRORS

PICNIC has been developed to account for the heterogeneity of the geosphere at two spatial scales. At the large-scale, transport in a network of so-called legs is considered (Fig. 1, top), between the repository and the next highly conductive feature (hcf). This goes beyond the geosphere modelling in the Kristallin-I study, where chiefly transport in a single leg with one-dimensional matrix diffusion (1D-MD) into a limited homogeneous planar or cylindrical rock domain was considered. Additionally, PICNIC has an increased flexibility to consider the small-scale heterogeneity of the geosphere; using the cross-section of the legs, the wallrock accessible for matrix diffusion is entered easily in a geometrical and flexible way to the code (Fig. 1, bottom).

To deal with this wide application range (Table 1), a fast and efficient hierarchical linear response method in the Laplace domain is used. Table 2 shows the flow scheme of PICNIC in which problem definition is followed by a "Russian doll" structure (1–10). This flow scheme relies on the linearity of the processes and on the fact that all processes only act locally. Matrix diffusion (level 1) acts locally at one position in the leg and locally at one value in the Laplace domain. Note that analytical relations are implemented for the rock matrix response (1) of the two rock matrix geometries considered in the Kristallin-I study. The increased flexibility for different rock matrix geometries is made by using an embedded finite element method. The effects of advection (2) and micro-dispersion (3) in the legs can be separated in the eigenvalues of the partial differential equations. The leg outlet boundary condition (4) influences only the pre-factors of the eigenvectors. The pathway initialization (5) is independent of all other levels. The pathway calculation (6) only makes use of (5) and of the leg response functions (4). The tree calculation (7) uses only the pathway result (6). The inverse Laplace transformation (8) is applied only to the results of the tree calculation (7). The source is convoluted in (9) with the tree response function (8). For multiple sources (10) the single source's results (9) are superimposed.

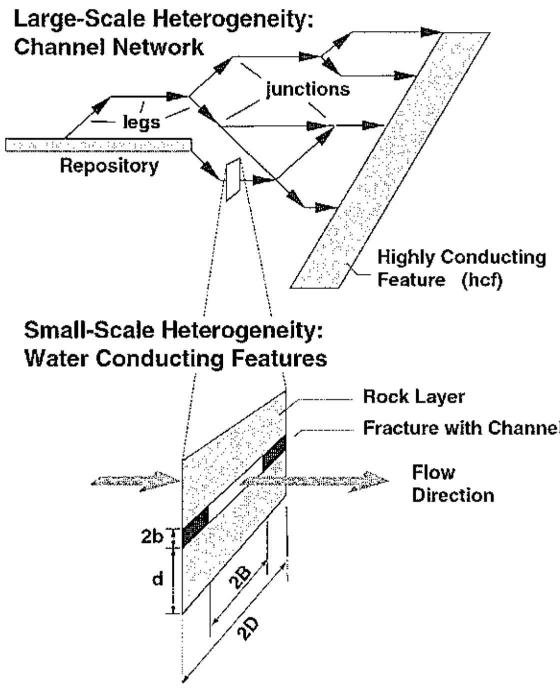

Fig. 1 Network representing the large-scale heterogeneity (top) and a cross-section of the flowpath representing the small-scale heterogeneity considered by PICNIC (bottom). The example rock matrix geometry conceptualizes water flow within channels and matrix diffusion as two-dimensional into a homogeneous rock layer.

Table 2 Condensed PICNIC flow scheme. Levels (1–7) work in the Laplace domain, and (9–10) work in the time domain. Level (8) is the inverse Laplace transformation.

Level		Problem definition: Russian doll structure
1	⇓	Matrix diffusion: embedded with analytical relations or with finite element method
2	⇓	Advection in leg
3	⇓	Micro-dispersion in leg
4	⇓	Leg outlet boundary conditions
5	⇓	Initialization of the pathway/tree; shape of source in "Laplace domain"
6	⇓	Pathway (sequence of legs between repository and hcf)
7	⇓	Tree (representing all pathways from a source to hcf)
8	⇓	Numerical inverse Laplace transformation (Talbot's method)
9	⇓	Convolution with "time-dependent" source
10		Multiple sources

From the structure of the code we estimate the possible "sources" of errors which have to be considered for a thorough verification. The calculation of the rock matrix response in level (1) should need only a few test cases when it is analytically implemented. When the embedded finite element method is used for the calculation of the rock matrix response, some level of error is inevitably generated. Its effect must be considered in detail. The calculation of the rock matrix response for nuclear decay chains is more complicated, because more processes interacting on different time scales are involved. In contrast to this, potential errors in the analytical transformations in the Laplace domain (in levels 2, 3, 4, 6 and 7, Table 2) should show up readily for simple tests. The calculation of the eigenvalues in level (3) can increase existing inaccuracies strongly for large Peclet numbers. The calculation of the leg response functions in (4) can also be a strong error amplifier, because of the exponential functions involved. The inverse Laplace transformation (8) is a key point for the reliability of the code. It means that the numerical integration in the complex plane is approximated as the sum of a finite series. The numerical convolution with the source in (9) is also not exact. However, it comes very late in the flow scheme, and its inaccuracies are not amplified. Also the superposition of the nuclide flow for multiple sources (10) should need only a few tests. As far as possible the "end product", i.e. time-dependent release curves, should be analysed and verified. Just verifying early individual code components (such as the finite element method in code level 1) is not sufficient because different code components work with varying degrees of success for different parameter regions, and especially because of the "error amplifiers" (3, 4 and 8) in the code.

VERIFICATION FOR ONE-DIMENSIONAL MATRIX DIFFUSION

The verification strategy presented here is based on the above considerations of the application range (Table 1) and the flow of control in PICNIC (Table 2). PICNIC is verified in a series of seven steps with increasing rock matrix complexity (Table 3); see Barten & Robinson (1999) for details. We start with 1D-MD into a homogeneous planar (step I, Table 3) and cylindrical rock matrix (step II), verifying the analytically implemented rock matrix response option. Cross-comparisons with RANCHMD for single legs are performed, showing excellent agreement of both codes. For verification of the network capability in PICNIC, a sequence of RANCHMD calculations for each individual leg in the network are combined to obtain the nuclide release of the network. The agreement with this so-called "assembled RANCHMD" result is excellent. Based on the internal structure of the code (Table 2) we can infer that these two steps have verified the capabilities of PICNIC to deal with transport in a pathway and a network of legs, to deal with different leg outlet boundary conditions, and to handle single or multiple sources of different shape, cf. Table 1.

The further verification, for the embedded finite element method, concentrates chiefly on the transport of single nuclides and nuclide decay chains in single legs. "Discretization tests" considering different refinements in the finite element mesh for calculation of the rock matrix response are generally used to indicate the accuracy of the code in verification steps III to VII.

Different geometries for 1D-MD are considered in steps III to V. In step III the embedded finite element method in PICNIC is verified to deal with a simple homogeneous planar layer of rock matrix, by comparison with the PICNIC option with the analytically implemented rock matrix response (considered in step I). The excellent

Table 3 PICNIC verification scheme. C: comparison with other code; K: consistency test; P-I: comparison of finite element with analytically implemented option in PICNIC; R: consistency check of different discretizations in the finite element option in PICNIC ("discretization tests"); S: test of stationary behaviour. "S" in step VI represents the comparison with the ADINA code presented below.

Step	Rock matrix geometry	Single leg: single nuclide	decay chain	Pathway: single nuclide	decay chain	Network: single nuclide	decay chain
I	1D-MD planar geometry	C,S,K	C,K	C,K	C,K	C,K	C,K
II	1D-MD vein geometry	C	C				C
III	1D-MD single layer	P-I,S,K,R	P-I,R			P-I,R	P-I,R
IV	1D-MD double layer	C,S,K,R	C,R			K	
V	1D-MD heterogeneous	C,R	C,R	C,R	C,R	C,R	C,R
VI	2D-MD single layer	S,K,R	K,R			R	R
VII	2D-MD heterogeneous	K,R	K,R				

agreement with the latter indicates the accuracy of the finite element method for this type of geometry. The shapes of the relative difference functions act as "calibration curves" for the more complicated rock matrix geometries.

For 1D-MD into a two-layered rock matrix (step IV) the steady state nuclide flow of a single nuclide agrees very well with the analytical result (Barten *et al.*, 1998). For this geometry, recently a cross-comparison to the code RIP (Miller & Kossik, 1998) was possible for the full time-dependent behaviour.

For 1D-MD into two independent homogeneous areas of rock matrix (step V), very recently a cross-comparison to the PAWorks/LTG code (Dershowitz *et al.*, 1998) was possible also. For 1D-MD into two independent two-layered areas of rock matrix a cross-comparison with the RIP code was performed. RIP and PAWorks/LTG use numerical Laplace transformation methods, which differ from the method applied in PICNIC, to consider transport in networks in combination with different geometries for 1D-MD. With both codes, the agreement of PICNIC for the time-dependent behaviour is very good. The small differences slightly increase with the complexity of the rock matrix.

VERIFICATION FOR TWO-DIMENSIONAL MATRIX DIFFUSION

For two-dimensional matrix diffusion (2D-MD) in steps VI and VII, no analytical solution for the rock matrix response is available, nor is a code available for cross-comparison of the time-dependent behaviour. (Note that 2D-MD means spatially three-dimensional transport in a leg, while 1D-MD means a spatially two-dimensional process.) Thus the verification for 2D-MD relies chiefly on the verification of the embedded finite element method for 1D-MD, on qualitative estimates, consistency checks and "discretization tests" in different parameter regions, both for single nuclides and nuclide decay chains. These tests are performed in step VI of Table 3 for 2D-MD into a homogeneous rock layer as depicted in Fig. 1 (bottom). For this rock matrix geometry the PICNIC result for the steady state release of a single nuclide is also verified quantitatively, as shown in the following example.

"Discretization tests" and consistency checks for 2D-MD into a two-layered rock matrix (step VII) show similar results to the single-layered case for 2D-MD. The same holds for 2D-MD into the rock matrix geometry of Fig. 1 (bottom), where the black areas in the fracture (with widths $D - B$) are assumed to be also available for matrix diffusion.

EXAMPLE FOR TWO-DIMENSIONAL MATRIX DIFFUSION INTO A HOMOGENEOUS ROCK MATRIX LAYER

For 2D-MD into a homogeneous rock matrix layer (step VI in Table 3) the PICNIC result for the steady state release of a single nuclide is also verified quantitatively for transport in a single leg. Figure 1 (bottom), gives the leg cross-section for this type of rock matrix. This rock matrix geometry conceptualizes that water flows through a fracture with aperture $2b$. Part of the fracture is filled with impervious rock (black areas) and the water flows in open channels through the fracture plane. A rock layer (shaded area) of thickness d, available for matrix diffusion, is situated below and above the fracture. The width of the channel is $2B$, and the width of the available rock layer is $2D$. Such a geometry approximates the geometry of cataclastic zones observed in the crystalline basement of northern Switzerland (Fig. 10-7 in Thury *et al.*, 1994) more realistically than the very conservative approximation of 1D-MD (i.e. $D = B$), which was applied in Kristallin-I.

The influence of the width $2D$ of the altered wallrock on nuclide transport in a cataclastic zone is analysed for a constant source (Fig. 2(a)). The nuclide release strongly decreases with increasing width, $2D$, of the rock layer, indicating the relevance of 2D-MD in performance assessment. There is, however, no code available for comparison of the time-dependent behaviour. PICNIC calculations with different resolutions of the embedded finite element method (i.e. "discretization tests") are in very good agreement over the whole time range and for all widths ($2D$) of the rock layer. The relative differences within different PICNIC calculations slightly increase with increasing rock matrix widths. For example, consider the steady state release (Fig. 2(c)) calculated in three different ways using PICNIC: the standard PICNIC result (squares in Fig. 2(c)), a result using a refined mesh (crosses), and additionally enforcing a local refinement of the mesh by sub-dividing the rock matrix into two layers (full lines). The relative differences from the latter are given in Fig. 2(b).

To get an independent result for comparison with PICNIC, we have also calculated the rock matrix response using the finite element code ADINA (ADINA, 1992). The steady state release is derived from the numerically calculated rock matrix response (Fig. 2(c)). This is done using analytical relations similar to Barten *et al.* (1998), where 1D-MD into a two-layered rock matrix was considered. While PICNIC appears slightly to underestimate the release, ADINA appears to overestimate it. With refined meshes, as expected, the results of both codes are even closer (Fig. 2(b)). This quantitative agreement of both codes is most important for the verification of PICNIC for 2D-MD.

These results together with the detailed "discretization tests" for pulse-like sources, indicate that refined finite element meshes should be used in PICNIC for some high demand applications. Altogether PICNIC shows up as a reliable code for these 2D-MD cases also, and can be applied with confidence in performance assessments and modelling of transport experiments.

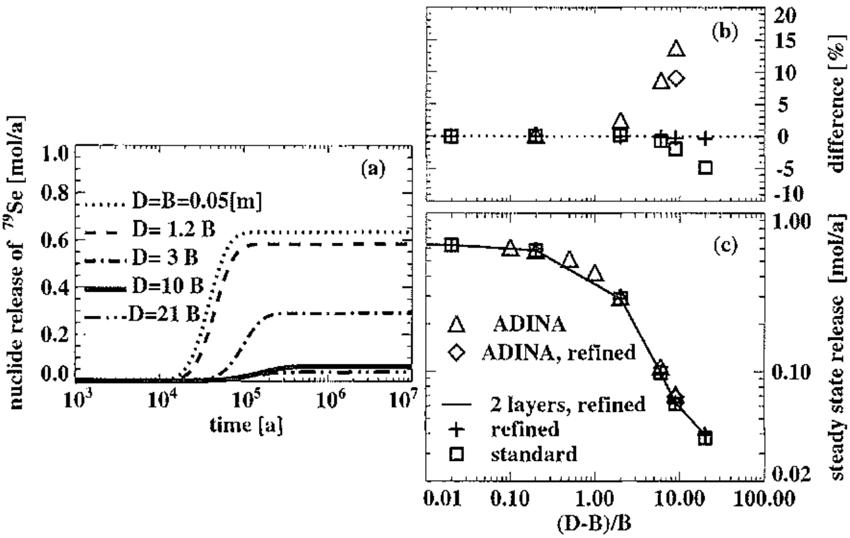

Fig. 2 (a) Release curves of the nuclide ^{79}Se for a single leg with different rock layer widths (2*D*) plotted for a constant source of 1 (mol year^{-1}). The dependence of steady state release on the rock layer width is given in (c); three different resolutions in PICNIC and a result derived from ADINA calculations are compared. For $D = 21B$ an additional ADINA calculation with a refined mesh is performed. (b) shows the relative differences from the highest resolution PICNIC result.

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