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Abstract

In the **C**olloid **F**ormation and **M**igration (CFM) Project at the Grimsel Test Site an experiment has been planned in order to study the generation of bentonite colloid and colloid facilitated radionuclides transport in a low gradient groundwater flow. During the first phase of this project a series of tracer tests have been performed to evaluate suitable flow fields for long-term colloid migration experiments within the fractured shear zone. The tracer tests with uranine have been accompanied by numerical modelling to support the in situ measurements. The overall objective of this modelling work is to understand the flow path and the relevant transport processes within the water-conducting shear zone, considering the low hydraulic gradients.

The numerical analysis was performed with the ADINA-F finite element code. The mathematical model is based on the Darcy's law for groundwater flow and the advection-dispersion equation for the uranine transport through a porous shear zone. For the numerical simulation a two dimensional model in the plane of the shear zone has been used. The computational domain considers the circular tunnel sealed with a surface packer, both injection wells and the extraction hole.

Both field data and modelling results provide a fairly consistent picture of the flow and transport characteristics in the shear zone at the planned CFM location. Furthermore, the simulation results match the experimental breakthrough curves fairly well and give confidence in the numerical model used. The estimated hydraulic and transport parameters from calibration work for two dipole fields show somewhat differences caused by natural heterogeneities in the hydraulic conductivity of the shear zone.

Modellierung von Tracer Experimente im Grundwasser einer Kluftzone im Grimsel Felslabor

Zusammenfassung

Im Rahmen des **C**olloid **F**ormation and **M**igration (CFM)-Projekts im Grimsel Felslabor wurde ein Versuchsfeld in einer Kluftzone des Kristallingesteins zur Untersuchung der Bildung und Migration von Kolloiden mit Radionukliden in Grundwasser eingerichtet. In der Vorbereitungsphase des Projekts wurde eine Serie von Feldexperimenten mit nicht-sorbierenden Tracern (Uranin) durchgeführt, um eine optimale Lokation (mit einem geringen hydraulischen Gradienten) für das geplante Hauptexperiment zu erörtern. Die Tracerversuche wurden durch Modellrechnungen begleitet, um die hydraulischen Verhältnisse und die Transporteigenschaften des Kluftzonematerials besser verstehen und interpretieren zu können.

Im vorliegenden Bericht werden Modellrechnungen mit dem Finite-Element-Programm ADINA-F durchgeführt. Das mathematische Modell basiert auf dem Darcy-Gesetz für die Beschreibung der Grundwasserströmung in der porösen Kluftzone und der advektiv-dispersiven Gleichung für den Tracertransport. Um die komplexen Fließbedingungen in dem Scherzonenbereich zu simulieren, wurde ein zweidimensionales Modell in der Kluftebene verwendet. Die Geometrie des Modells erfasst den Nahbereich der abgedichteten Versuchsstrecke durch einen Flächenpacker sowie die beiden Injektions- bzw. Extraktionsbohrungen.

Mit Hilfe dieses Modells konnte die zeitliche Entwicklung von Durchbruchskurven von Uranin zufriedenstellend reproduziert werden. Die wichtigsten Transportparameter des porösen Kluftmaterials an zwei Versuchsfeldern wurden bestimmt. Die beiden Bereiche unterscheiden sich deutlich in den hydraulischen Eigenschaften.

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1 Introduction

Crystalline rocks such as granite have been extensively investigated as a potential host rock for nuclear waste disposal. The crystalline rock matrix is nearly impermeable and the groundwater flows predominantly through discrete features such as fractures filled with porous material. Such features are thus likely to provide the primary pathway for the migration of radionuclides from an underground repository to the biosphere. In order to predict the movement of radionuclides, the processes involved must be understood and quantified. For this purpose, laboratory tests, field experiments supported by numerical models are needed.

The generation of colloids from a bentonite-based engineered barrier system and their influence on radionuclide migration is currently investigated in the frame of the in-situ experiment programme: The Colloid Formation and Migration Experiment (CFM) conducted in the Grimsel underground laboratory (Grimsel Test Site, GTS, NAGRA, Switzerland) [1]. The aim of this international project is to study the migration of radionuclides and colloids through a fractured shear-zone in crystalline rock under in situ conditions such as low hydraulic gradients i.e. low ground water velocity. In order to characterise the initial conditions for the planned long-term experiment and to provide a data set for the calibration of the local groundwater model, several dipole experiments using uranine as a tracer have been performed.

This report presents a summary of the modelling work performed by the Institut für Nukleare Entsorgung (INE) to investigate the long-term flow and the transport of the tracers in the fractured shear zone at two different locations where in-situ colloid and radionuclides migration experiments are planned to take place. The calculations were carried out using the finite element code ADINA-F [2]. The mathematical model was based on the Darcy's law and the conservation of mass for groundwater flow and the advection-dispersion equation for uranine transport. The main objectives of the numerical analyses are to estimate the flow and transport parameters from tracer test breakthrough curves.

2 Flow and transport equations

Assuming that fluid flow in the fracture is laminar and isothermal, the momentum balance equation for fluid flow can be simplified to the well-known Darcy's law [3]. For the 2D incompressible flow in a porous medium the governing equation is given by

$$\mathbf{V} = -1/\mu \mathbf{K} \cdot \nabla P \tag{1}$$

here $\mathbf{V} = [v_y,\ v_z]^{\mathrm{T}}$ is the vector of the components of averaged groundwater velocity in the $y,\ z$ directions, μ is the dynamic viscosity coefficient, $\mathbf{K}$ the intrinsic permeability tensor and ∇P the water pressure gradient.

In this report only the transient transport of conservative tracers through a saturated porous medium is modelled, therefore only advection, diffusion and dispersion are relevant processes.

Advection: The contaminants are travelling at the same rate as the average linear velocity of the ground water. The average linear velocity is not equal to the Darcy velocity but can be calculated by dividing the Darcy velocity components by the effective porosity η_e.

Dispersion: The dispersion is a phenomenon coupled to heterogeneities of flow velocities on all scales. The different flow paths and apertures create differences in the path length and velocities which cause dilution when they mix again. An important feature is the large scale heterogeneities of permeability distribution which causes spreading in all directions. The kinematic dispersion accounts the complex features of the flow paths that cannot be modelled with the concept of average velocity. The dispersion term in the transport equation is mathematically described with Fick's law.

Molecular Diffusion: The molecular diffusion is a process by which molecules move from areas of high concentration to areas of low concentration. This phenomenon can also be modelled by Fick's law. The molecular diffusion takes place even the water flowing or not. If the flow velocities are high then the effect of molecular diffusion is small compared to the advection and the dispersion.

Combining the molecular diffusion and the dispersion to a hydrodynamic dispersion $\boldsymbol{D}$ and adding a source/sink term, S, the transport equation yields the following balance equation:

$$\partial C/\partial t = \nabla \cdot \left(\boldsymbol{D}\,\nabla C - \eta_e \mathbf{V}\,\nabla C\right) - S \tag{2}$$

where C is the concentration of the species in the pore fluid and R is the retardation factor for linear sorption in the porous material. $\boldsymbol{D}$ is the tensor of hydrodynamic dispersion. The coefficients of hydrodynamic dispersion are evaluated using the equation:

$$D_{kl} = (D_o + \alpha_T \mathrm{V})\, \delta_{kl} + (\alpha_L - \alpha_T)\, (v_k\, v_l) / \mathrm{V} \qquad (3)$$

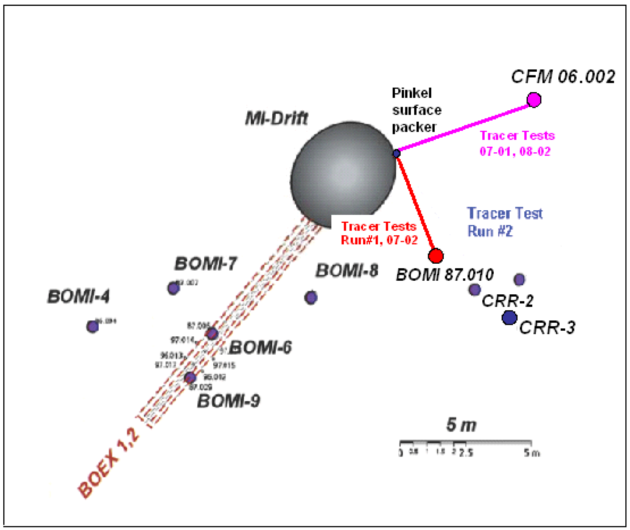
where D_o *is* the coefficient of molecular diffusion, α_L, α_T are the longitudinal and transverse dispersion lengths, δ_{kl} is Kronecker's delta, v_k , v_l are the components of the average groundwater velocity, V is the magnitude of the average groundwater velocity and the set (k, l) range over the indices y, z.

3 Numerical modelling of the tracer tests

The numerical analysis was performed with the general purpose code ADINA-F which offers a wide range of capabilities. In our study ADINA-F was used for calculation of fluid flow coupled with the mass transport in a saturated, porous medium. An iterative solution procedure for the transient solute transport was used.

In the first phase of the CFM project, different tracer tests with uranine as conservative tracer were performed in the low gradient flow field within the shear zone at the planned experiment location. The goal of the analysis of the tracer tests was to estimate the hydraulic and transport parameters of the fractured shear zone by fitting model outputs to measurements.

Prior to the tracer tests, the experimental tunnel was equipped with a 3m-diameter surface packer system. The scope of this packer was to avoid uncontrolled flow rates towards the drift, to reduce the hydraulic gradient in the shear zone and to achieve longer tracer travel times. In this contribution the tracer tests performed in two different dipoles were analyzed numerically. Fig. 1 shows the location of the injection boreholes CFM 06-002 and BOMI 087.010 respectively and the extraction point (Pinkel) at the surface packer in the plane of the shear zone around the experimental



drift.

Fig. 1: Location of the tracer tests used for model calibration and the different observation

boreholes in the plane of the shear zone around the experimental drift (source Nagra)

Tracer Test	**Characteristics**
Run #1 between BOMI 87.010 and Pinkel surface packer Distance 4 m	Injection flow rate: 4.5 ml/min Injected tracer volume 200ml Uranine concentration 5.6 ppm Outflow rate 653 ml/min (from Pinkel and fissure)
Run 07- 02 between BOMI 87.010 and Pinkel surface packer Distance 4 m	Injection flow rate: 3.4 ml/min (60 min) and 120 ml/min Injected tracer volume 204ml Tracer mass 2 mgr Recirculation flow rate 120 to130 ml/min Outflow rate 120 ml/min
Run 07- 01 between CFM 06.002 and Pinkel surface packer Distance 6 m	Injection flow rate: 9.18 ml/min Injected tracer volume 280 ml Tracer mass 14 mgr Recirculation flow rate 80 ml/min Outflow rate 165 ml/min
Run 08 - 02 between CFM 06.002 and Pinkel surface packer Distance 6 m	Injection flow rate: 10 ml/min Injected tracer volume 280.2 ml Tracer mass 15.4 mgr Recirculation flow rate 25 ml/min Outflow rate 165 ml/min (160 ml/min from annular gap)

Tab. 1: Summary of tracer tests used for model calibration, Ref. [4]

3.1 Calculation model

In this study, it was assumed that the groundwater flow and the solute transport take place only in fractures filled with fault gouges, and the shear zone at the test location is plane. However, the model represents a planar confined porous media with a constant porosity and an anisotropic permeability. The initial and boundary conditions assumed in the calculation are shown in the Fig. 2. The ground water flow in the model domain was calculated on the assumption of impermeable top and bottom boundaries and a uniform, regional flow from left to right, with a velocity of 10 m/year. The uranine concentration curves which were measured at the injection hole in every test have then been used as input data in the model calculations.

The present finite element model extents the relatively simple model used in an early stage of the CFM project. The 20m by 12m domain including the drift and the injection and extraction holes was meshed by 10564-four-node planar elements. The shear zone is assumed to be 1cm in thickness. The entire mesh and a detail of the mesh near the wells are shown in the Fig. 3. The groundwater and the uranine were injected at one of the boreholes BOMI 87.010 or CFM 06.002 with flow rates indicated in Tab. 1 and extracted at the surface packer at rates given also in the table above.

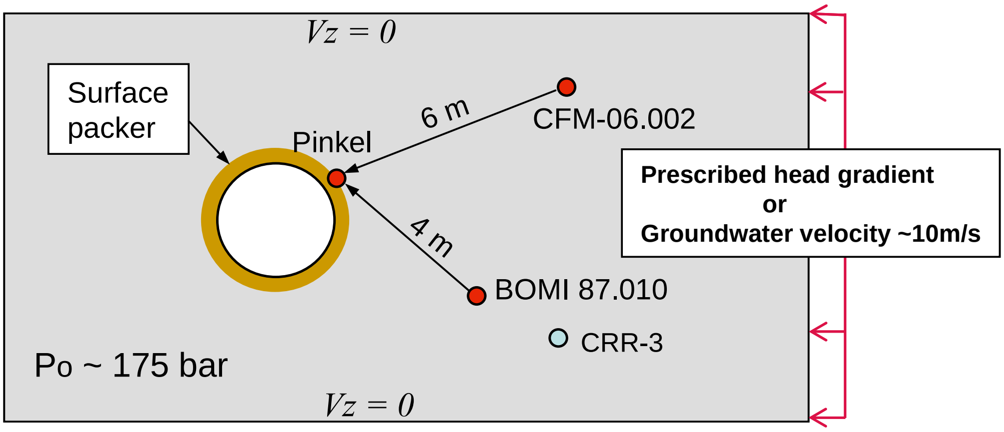


Fig. 2: Definition of the model boundary condition for simulation of tracer tests

3.2 Results and discussion

The calculation starts with the modelling of the steady-state groundwater flow field in each dipole experiment. After these conditions were established, the injection of the uranine solution was simulated. The uranine concentration was measured online in order to determine the input functions and then used directly in this numerical analysis.

The simulation of the uranine Run # 1 and test 07-02 (Refs. [5, 6]) have been used for the calibration of the numerical model for the Dipole 2 (between BOMI-87.010 and Pinkel surface packer) and the uranine tests 07-01 and 08-02 (Refs. [4, 7]) for the Dipole 1, respectively. Both dipoles are proposed as potential location for the final long-term radionuclide migration experiment.

3.2.1 Simulation of the uranine breakthrough curves in Dipole 2

In the tracer test Run #1 the uranine was injected at the borehole BOMI 87.010 and recovered at the Pinkel surface packer and at a fissure near this packer. The uranine concentration measured at the injection borehole is presented in Fig. 4. The calculated and measured uranine breakthrough curves at the outflow borehole are plotted in Fig. 5. As can be observed the simulation matches the concentration peak at the extraction hole quite well. However, the comparison of calculation results in the tailing part shows some differences. The material parameters used for this analysis are given in Tab. 2.

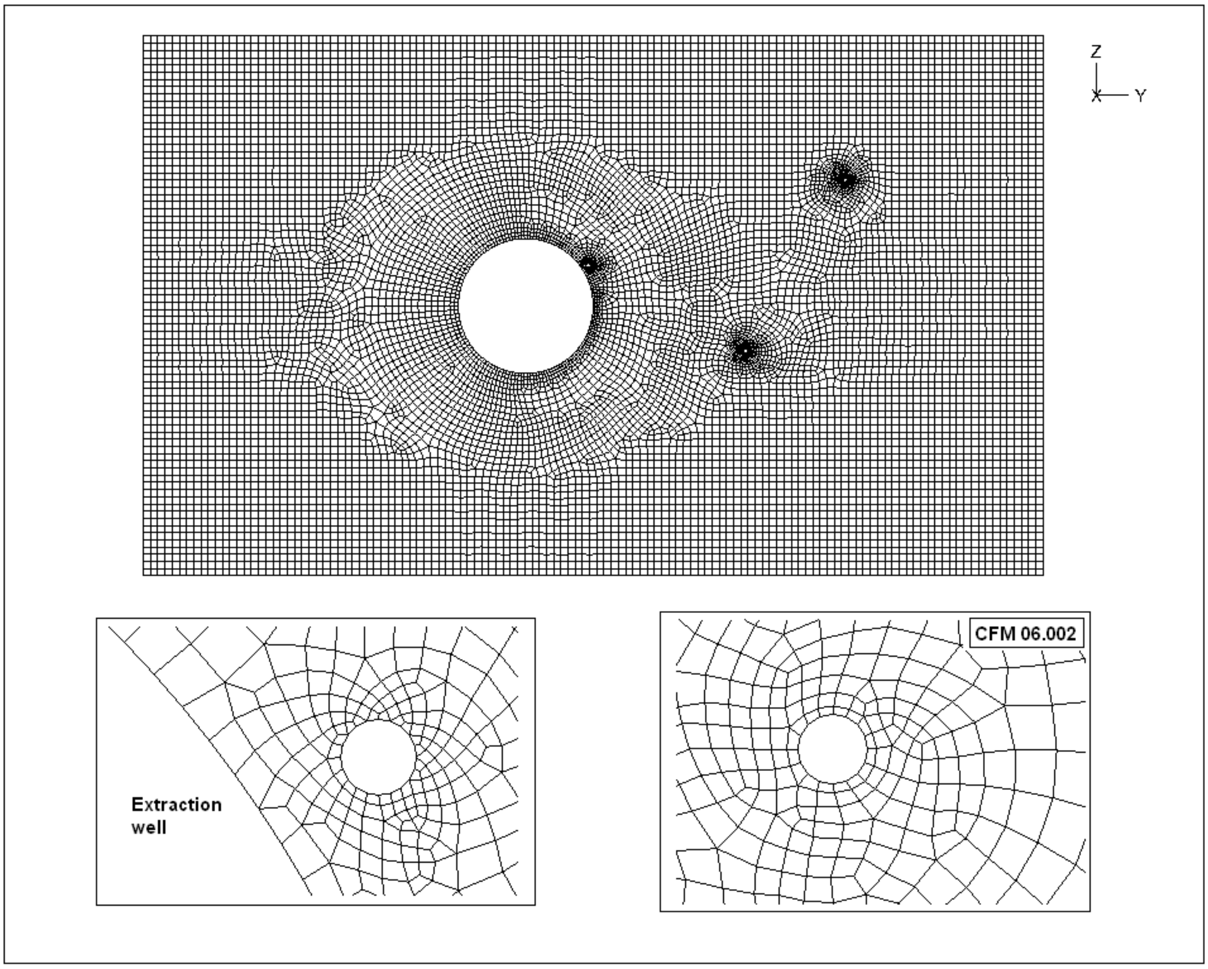


Fig. 3: Finite element model used for calculation of tracer tests and detail of the mesh near the boreholes; Extension of the model: 20x12 m^2

In the next step the uranine test 07-02 at relatively low outflow (120 ml/min) has been modelled. For this test the uranine concentration measured at the injection borehole is shown in Fig. 6. Figure 7 depicts the calculated and measured uranine break-through curves at the extraction hole (Pinkel). As can be seen, the model produces a reasonable fit to the experiment. There is clearly a good agreement between both curves regarding in-peak arrival time and the tail. The long tailing seems to be in-duced by progressive release of the tracer late in the injection interval. The evolution of computed uranine concentration in the shear zone is presented in Fig. 9. The plots show that the main flow pathway of the tracer is toward the extraction hole but a small amount of tracer is passing around the drift. This is due to the diffusion and dispersion processes taking place during the long travel time in the weak dipole test.

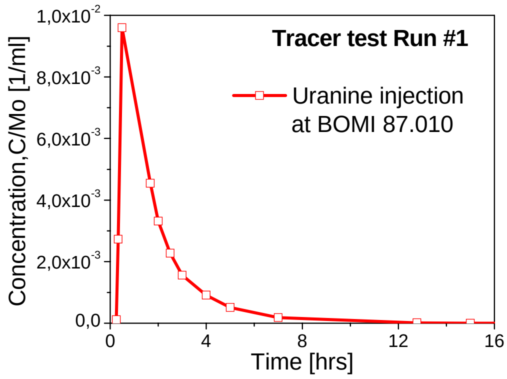


Fig .4: Measured uranine concentration for Run #1 at the injection well, BOMI 87.010

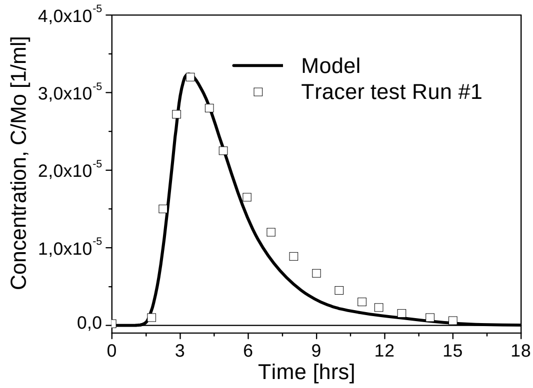


Fig. 5: Fitted and measured breakthrough curves for uranine in Dipole 2, Run #1

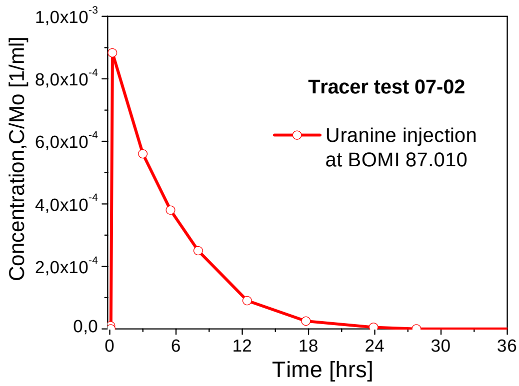


Fig. 6: Experimental input concentration of the uranine for run 07-02 (Dipole 2)

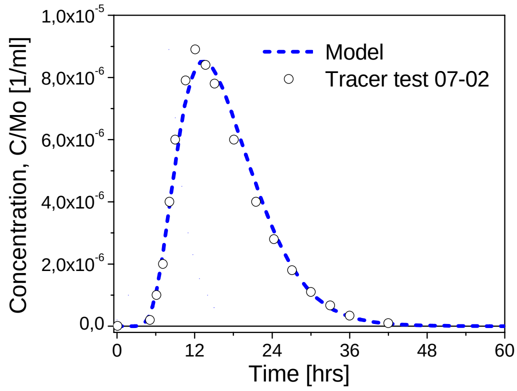


Fig. 7: Calculated and measured break-through curves at the extraction well (tracer mass recovery about 86%)

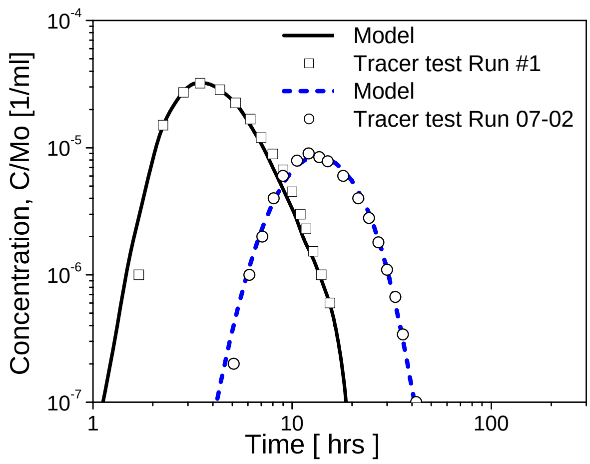


Fig. 8: Comparison of measured and calculated breakthrough curves for tracer tests Run #1 and 07-02 (presentation on logarithmic scales)

The results suggest that the use of an anisotropic hydraulic permeability of the shear zone, which was successfully applied to fit earlier tracer experiments [8], does not work in this case. However, it seems that the heterogeneity of the shear zone material with respect to porosity and permeability in the model domain will influence the transport processes under the low or natural hydraulic gradients.

The hydraulic parameters obtained from preview simulation of Run #1 (same dipole but different flow rates) were used firstly. However, it was necessary to perform further adjustments of these parameters due to the new test conditions (i.e. smaller pumping and extraction rates) to be able to fit the measured breakthrough curve. The fit of the model to the both experimental breakthrough curves in the Dipole 2 is presented again on logarithmic scales in Fig. 8. The calibrated input parameter sets are given in Tab. 2.

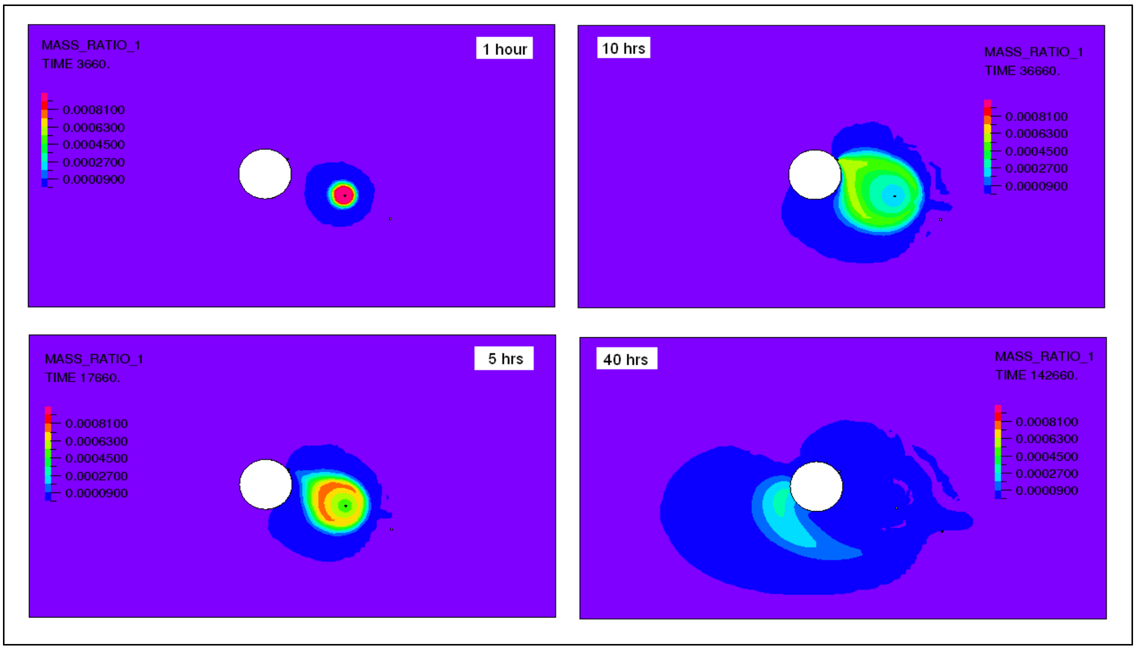


Fig. 9: Distribution of the uranine concentration after different times

3.2.2 Simulation of the uranine breakthrough curves in Dipole 1

In the tracer tests 07-01 and 08-02 the uranine was injected at the borehole CFM 06.002 and recovered at the Pinkel surface packer. These tests are performed in a restricted flow field at outflow rates of about 165 ml/min. The uranine test 08-02 runs subsequent to the first homologue tracer test (run 08-01). The shape of the both experimental breakthrough curves is quite different due to technical problems during the test 07-01. After this experiment the injection equipment was changed. The uranine injection functions of both tests are presented in Fig. 10. The comparison of calculated and measured breakthrough curves is illustrated in Figs. 11 and Fig. 12. The double peak observed in the concentration breakthrough curve of the test 07-01 seems to be induced by the encountered technical problem. This kind of peak was not observed by the subsequent tests (i.e. homologue test, 08-01 and the tracer test 08.02)

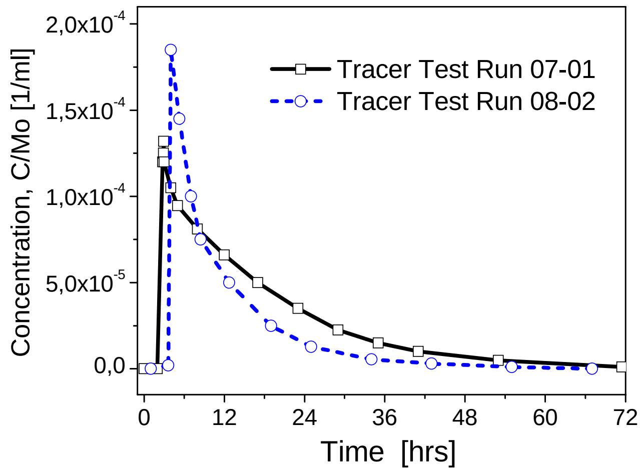


Fig. 10: Measured uranine injection functions for two different tests in the Dipole 1.

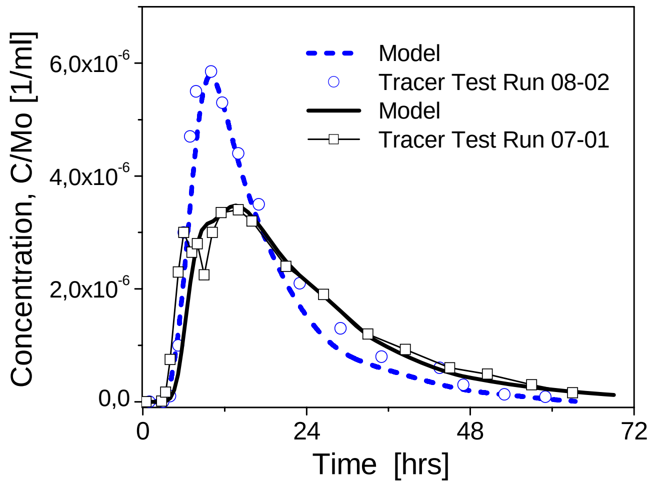


Fig. 11: Comparison of measured and calculated breakthrough curves for both tracer tests in the Dipole 1 flow field

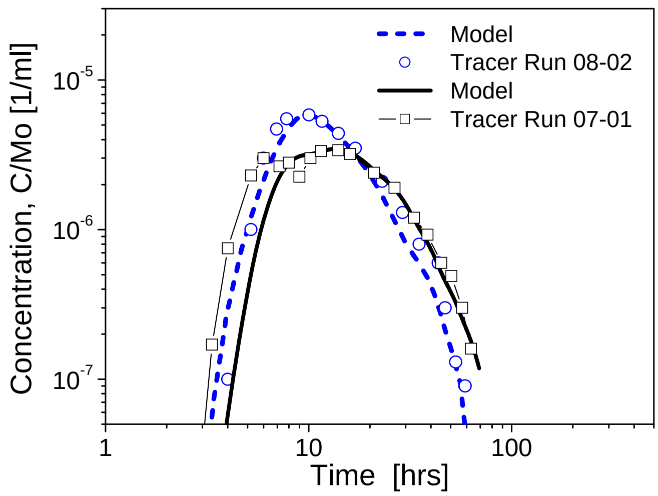


Fig. 12: Comparison of measured and calculated breakthrough curves for tracer tests Run 08-02 and Run 07-01 (logarithmic presentation)

	Dipole 2		Dipole 1
	Run #1	**Run 07- 02**	**Run 07- 01 and 08- 02**
Flow porosity	0.1	0.1	0.12
Horizontal permeability (m^2)	2E-11	1E-11	2E-09
Vertical permeability (m^2)	1E-11	1E-11	1E-09
Longitudinal dispersion (m)	0.005	0.005	0.002
Transversal dispersion (m)	0.0005	0.0005	0.0002
Diffusion coefficient (m^2/s)	2E-11	2E-11	2E-11

Tab. 2: Comparison of hydraulic and transport parameters used to model the tracer tests

In the model calculation, after 30min from the start of uranine injection a 20 % higher inflow rate was assumed. The double peak has been nearly reproduced and the calculated breakthrough curve is similar to the measurements.

For the tracer test 08-02 the transport parameters have been kept the same as for run 07-01. In this case the model reproduces the peak height position and width, as well as the shape of the tail. The computed piezometric head and the evolution of uranine concentration in the shear zone for the tracer test 08-02 are illustrated in Fig. 12. The plots show that the mean flow pathway of the tracer is toward the extraction well.

Regarding the all hydraulic and transport properties obtained from this calibration work on tracer tests it can be concluded that the area below the drift (Dipole 2) is less permeable (transmissive) as the region around the dipole 1. These results confirm the Nagra's highly heterogeneous model of the hydraulic transmissivity as already described in Ref. [9].

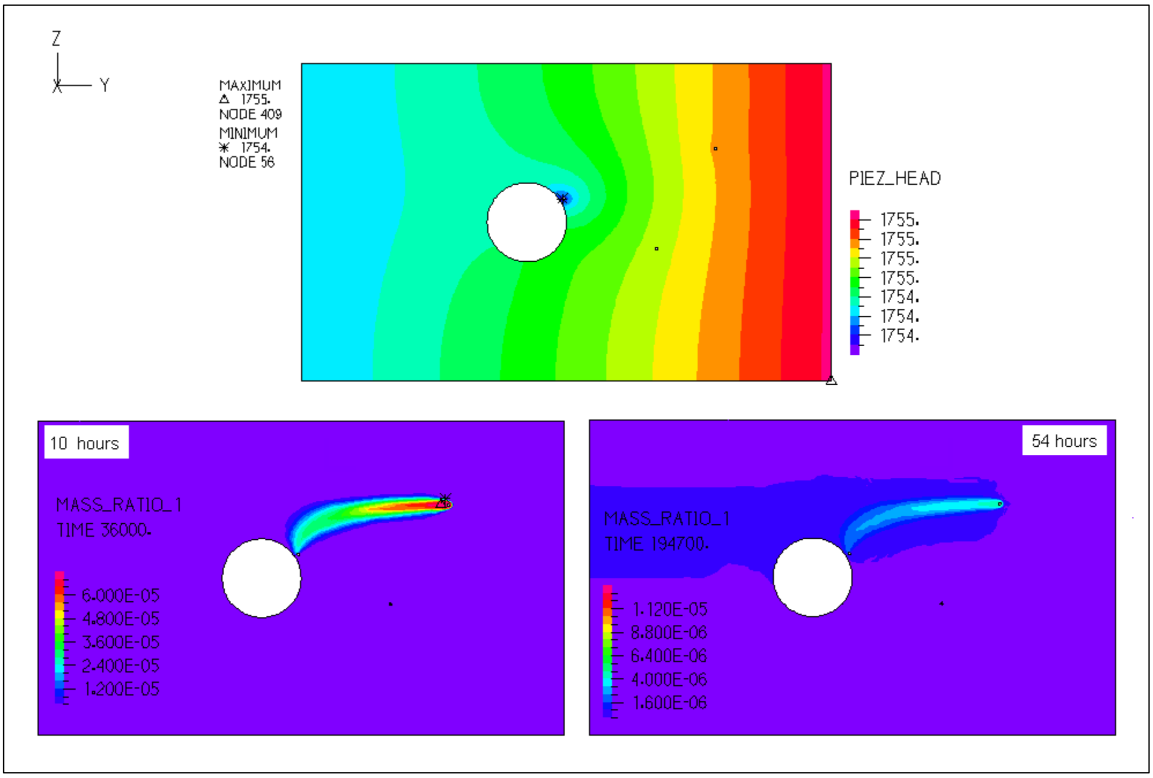


Fig. 13: Distribution of piezometric head and uranine concentration 10 and 54 hours after the start of tracer injection

4 Conclusions

During the first phase of the CFM project several conservative tracer tests were performed at two different locations. The measured uranine breakthrough curves have been then used for model calibration. Subsequently, the calibrated model has been compared with independent measurements.

The field data and the modelling results provide a fairly consistent picture of the flow and transport characteristics in the shear zone at the planned CFM experiments. The 2D numerical model considers uniform but anisotropic permeability and constant porosity of the shear zone. Therefore, the estimated hydraulic and transport parameters must be considered as an approximation of the real structure which indicates heterogeneities in the hydraulic conductivity. For all that, it appears that the model provides a good database to assist in the planning of future complex calculations.

In the next project step, further work is required to explore how the uncertainties on parameter estimation and the subsequent predictions at lower hydraulic gradients are affected by the choice of the present conceptual model. However, the test 08.01 with homologue radionuclides will be simulated using the transport parameters obtained by fitting the uranine tests. Furthermore the improvement of the large scale hydraulic model taking into account the heterogeneous hydraulic conductivity of the shear zone will be performed.

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