GAS TRACER TRANSPORT IN TWO-PHASE FLOW FIELD: NUMERICAL SIMULATIONS AND FIELD EXPERIMENTS AT THE GRIMSEL TEST SITE (GTS), SWITZERLAND

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INTRODUCTION

During Phase IV of the R&D program at the Grimsel Test Site (GTS), NAGRA (National Cooperative for the Disposal of Radioactive Waste) has been investigating the two-phase flow (TFP) behavior in fracture zones (Marschall et al., 1997). In the proposed repository for low-level/intermediate-level waste (LLW/ILW), gas will be generated by anaerobic corrosion of metals and by chemical and microbial degradation of organic substances. Waste-generated gas from such an underground repository will escape mainly through preferential pathways (e.g., shear zones, fractures) in the host rock, which is initially fully water-saturated. To better understand two-phase flow and transport behavior in shear zones, extensive investigations have been conducted in the FRI zone (Fracture Rock Investigation zone) at GTS (Fig. 1). In addition to hydraulic- and gas-injection tests, the TPF investigations also included the design and implementation of gas tracer tests in the field and in numerical models.

Gas tracer tests were conducted in a two-phase dipole flow field between two boreholes intersecting the initially fully water-saturated fracture zone. Two gas tracers (Helium and Xenon), characterized by different solubility, were injected under approximate steady-state, two-phase flow conditions in the dipole field. The potentially different tracer breakthrough is an indication not only of the mass transfer properties between gas and liquid, but also of the two-phase flow parameters affecting the saturation distribution in the dipole field.

The scope of Phase IV of the TPF Investigation Program at GTS was to develop the experimental procedure for conducting gas tracer tests. Furthermore, the field experiments were used to test the numerical models and the analysis capabilities for gas tracer tests and to develop a conceptual understanding of two-phase flow and transport in fracture zones. This paper briefly describes the field experiments at the FRI zone and the numerical implementation of the tests. Based on the simulations of the field experiments, design simulations were performed in preparation of the next investigation phase of gas tracer testing at GTS.

FIELD EXPERIMET

Figure 1 shows the location of the different test boreholes and intervals within the FRI zone. In addition to the two main boreholes BOTP 95.001 and BOTP 95.002 with injection intervals I2.2 and extraction interval I1.2, respectively, additional monitoring boreholes were completed in the FRI zone. They were used during the hydro- and extended gas threshold pressure tests (EGTPT), which were conducted to determine the hydraulic and two-phase flow properties of the shear zone during an earlier investigation phase (Wyss, 1996, Croise & Senger, 1996). In the current investigation phase, the injection and extraction intervals I2.2 and I1.2 for the tracer test configuration are 0.66 m apart. Also indicated in figure 1 is the location of the new boreholes, which are planned for the next investigation phase and are as much as 4 m away from the main boreholes.

In addition to monitoring the pressure in the injection borehole, the gas tracer test involved measuring the flow rates of gas and water. More importantly, the gas tracers have to be detected in the extraction interval. This required separating the gas-water outflow from the extraction interval in order to continuously analyze the tracer concentration. For this, two separate mass spectrometers were employed to measure the He and Xe concentrations. The details of the experimental procedure is given in Bühler et al. (1997). In this experimental setup, the concentration of gas tracers dissolved in the liquid phase were not measured.

The pressure response in the injection well during the initial gas injection test for establishing the two-phase dipole flow field is shown in Figure 2, based on a constant gas injection rate of 50 ml(STP)/min in the injection well and keeping a constant pressure at the extraction interval of 0.5 bar. The data show a steep pressure increase until gas breakthrough in the extraction interval occurs, after which the injection pressure declines to level off at approximately 3 bar.

For the subsequent gas tracer test, the total gas injection rate remained at 50 ml(STP)/min; the gas, however, consisted of 95% N_2 and 5% He and Xe in equal amounts. The gas tracers were injected for a total of about 111 hours (4.0E+5 sec) followed by continued injection of 100% N_2. Figure 2 shows the breakthrough curves for the He and Xe tracers in the gas phase at the extraction interval. The initial breakthrough of both tracer occurs about 12 minutes after tracer injection started without noticeable differences between the two tracers. Similarly, concentrations of both tracers reach a plateau within a few hours and show similar tailing after the tracer injection stopped.

MODELING APPROACH

The numerical simulations were performed with the EOS7R module, which was developed to provide radionuclide transport capabilities for TOUGH2 (Oldenburg & Pruess, 1995). EOS7R simulates flow of two phases (air and water) with transport of five components: (1) water, (2) brine, (3) parent radionuclide, (4) daughter radionuclide, and (5) air. The radionuclide components can consider first-order decay and may adsorb onto the solid grains. They can be in either the gas or liquid phase, that is, volatile radionuclides can be dissolved in the aqueous phase. Transport of the five components is by advection and molecular diffusion in both phases. EOS7R can be coupled with the dispersion module T2DMR taking into account hydrodynamic dispersion for 2-D rectangular grid geometry. To simulate a gas tracer test with EOS7R, the radionuclide components are represented by the gas tracers having the chemical properties of He or Xe (Table 1). In this case, decay and sorption of the component is set to zero.

The numerical simulations included both the gas injection into the fully water-saturated FRI zone, creating an approximate steady-state two-phase dipole field and the subsequent gas tracer test. For this purpose, a numerical model was constructed for the FRI zone represented by a 2-D cross-sectional model, whereby the thickness of the 2-D mesh corresponds to the inferred thickness of the shear zone. The test configuration was implemented in a rectangular mesh with refined grid spacing near the injection and extraction intervals. The grid orientation was such that the x-direction parallels the line segment through the injection interval and the extraction intervals. In the first model configuration gravitational effects were neglected. With this, the line segment through the injection and extraction intervals corresponds to a symmetry axis which is represented by a no-flow boundary in the numerical model. The borehole intervals are represented by a rectangular grid block with the actual test-interval volumes. Constant pressures are prescribed at the outer model boundaries to allow pressure dissipation across these boundaries during the gas injection test. In the second set of simulations for the design of the planned gas tracer test, where the injection and extraction intervals as much as 4 m apart, a similar mesh configuration was used; this time, the injection and extraction intervals are in the center of the model taking into account potential gravitational effects.

The hydraulic and two-phase flow parameters of the FRI zone used as input for simulation of the dipole gas injection and subsequent gas tracer tests are based on previous analyses of hydro- and extended gas threshold pressure tests in the injection zone I2.2 in borehole BOTP 95.002 (Wyss, 1996, Croise & Senger, 1996). The relevant input data for the simulations are summarized in Table 1. For the gas injection test establishing the two-phase dipole flow field and for some of the tracer test simulations, different two-phase parameter models were evaluated based on the results of the EGTPT in I2.2 (Croise and Senger, 1996): (a) Parameter set 1 is based on the van Genuchten model (vG/MG), characterized by significant phase interference, and (b) Parameter set 2 is based on a van Genuchten model (vG/M) with enhanced gas relative permeability ($k_{rg} = 1 - k_{rl}$).

Table 1. Relevant Input data for the different simulations

Parameter	**Values**	
Hydraulic data:	**Parameter Set 1**	**Parameter Set 2**
Permeability (k)	2.29E-15 m^2	8.13E-15 m^2
Compressibility (C)	1.51E-9 Pa^{-1}	1.51E-9 Pa^{-1}
Porosity	0.08	0.08
FRI-zone thickness (b)	0.018 m	0.18 m
Test-zone compressibility (C_{tz})	1.95E-8 Pa^{-1}	1.95E-8 Pa^{-1}
Initial pressure (P_i)	1.05E+5 Pa	1.05E+5 Pa
Prescribed pressure in I1.2	0.5 E+5 Pa	0.5 E+5 Pa
Two-phase parameter model:	**vG/MG-model**	**vG/M-model**
vG-parameter: m	0.583	0.583
vG-parameter: $\log_{10}(1/\alpha)$	6.6E+4 Pa	6.6E+4 Pa
Residual water saturation	0.23	0.23
Gas Injection:		
1. Phase (gas injection test)	Q(N2) = 50 ml (STP)/m; Q(air) = 9.902E-7 kg/s	
2. Phase (gas tracer test)	Q(N2) = 49.5 ml(STP)/min; Q(air) = 9.803E-7 kg/s Q(He) = 0.25 ml(STP)/min = 3.422E-10kg/s Q(Xe) = 0.25 ml (STP)/min =1.123E-8kg/s	
Tracer Data:	**He**	**Xe**
Mol. Weight	4.003 g/mol	131.3 g/mol
Density (STP at 20^0C, 1 bar)	0.1642 kg/m^3	5.387 kg/m^3
Molecular Diffusivity liq./gas ()	1.E-5/1.E-9 m^2/s	1.E-5/1.E-9 m^2/s
Solubility^2 (cm^3/cm^3-H_2O)	0.00865	0.168
Inverse Henry Constant (at 1 bar)	1.4708E-11 Pa^{-1}	9.37E-9 Pa^{-1}

SIMULATION RESULTS

The simulation results for establishing the two-phase dipole flow field are shown in Figure 2. The simulated pressures in the injection interval differ for the two parameter set, and show some differences to the measured pressures. The measured injection pressures level off at a much lower pressure compared with the simulation results based on parameter set 1, but is slightly higher than the simulation results based on parameter set 2 (Fig. 2). The distinct pressure change observed after about 100,000 sec could not be reproduced, which may be due to a sudden change in the gas injection rate.

The gas tracer simulations show overall similar tracer breakthrough curves in the extraction interval as those in the field experiment (Fig. 3). The simulation using parameter set 1 (vG/MG model) indicate that the first arrival of the He tracer occurs after about 10 min, which is in good agreement with the field observations, whereas the first arrival of the Xe tracer is somewhat delayed at about 30 min. The simulated tracer breakthrough curves in the gas phase show that during the injection period the relative concentrations of He are higher than of Xe. After tracer injection stopped, Xe concentration tend to be higher than He concentration (Fig. 3). The delayed breakthrough and the higher tailing of Xe is to be expected, because of the much higher solubility of Xe compared with He. Simulations results using parameter set 2 (vG/M model) are similar to those in Figure 3.

The field results did not indicate a distinct difference in the tailing between He and Xe. This is probably due to the small volume in the shear zone and the short flow paths for the tracer between the injection- and extraction interval. The numerical simulations reproduced the overall shape of the gas breakthrough curve, but indicated some differences between He and Xe; the latter showed some more tailing as one would expect from the higher solubility. The difference between the field test and the model is likely due to the assumption of local thermodynamic equilibrium at the grid-block scale. This may suggest that the effective solubility of tracer components is reduced due to diffusion-limited mass transfer at the interface between the gas and liquid phase. Local thermodynamic equilibrium at the grid-block scale cannot account for such microscopic processes; that is, the relatively coarse grid spacing and the close proximity of the test intervals may overestimate the solution of gas tracers.

As a result of the field experiment, a larger gas tracer test is planned at the FRI zone, where the injection and extraction intervals are as much as 4 m apart. In preparation of this next investigation phase, design simulations were performed for a larger dipole field. The design simulations show that for such a two-phase dipole flow field, the first arrival of the tracer occurs within 40 hours for Xe and about 5 hours for He, even with a relatively low gas injection rate of 25 ml(STP)/min. Over that long distance, the breakthrough curve for Xe is significantly different than for He (Fig. 4); Xe indicates significant tailing due to the higher liquid solubility of Xe than He. Also, the different parameter models (vG/MG and vG/M) show different breakthrough curves, even for the gas phase. This could be important for better constraining the two-phase parameter model in the fracture zone.

SUMMARY

The field experiments during Phase IV of the TPF program at the FRI zone at GTS demonstrated the feasibility of conducting and analyzing gas tracer tests in a fracture zone. Two gas tracers (He and Xe), having significant different solubility, were used to evaluate mass transfer between the gas and water phase and to characterized the two-phase flow conditions in fracture zones. Numerical simulations of the gas tracer test were performed with the TOUGH2 module EOS7R, which could reproduce the overall tracer breakthrough behavior observed during the field test. For the greater dipole flow field planned in the next investigation phase, the gas tracers indicate significant different breakthrough curves as a result of the different solubility of He and Xe.

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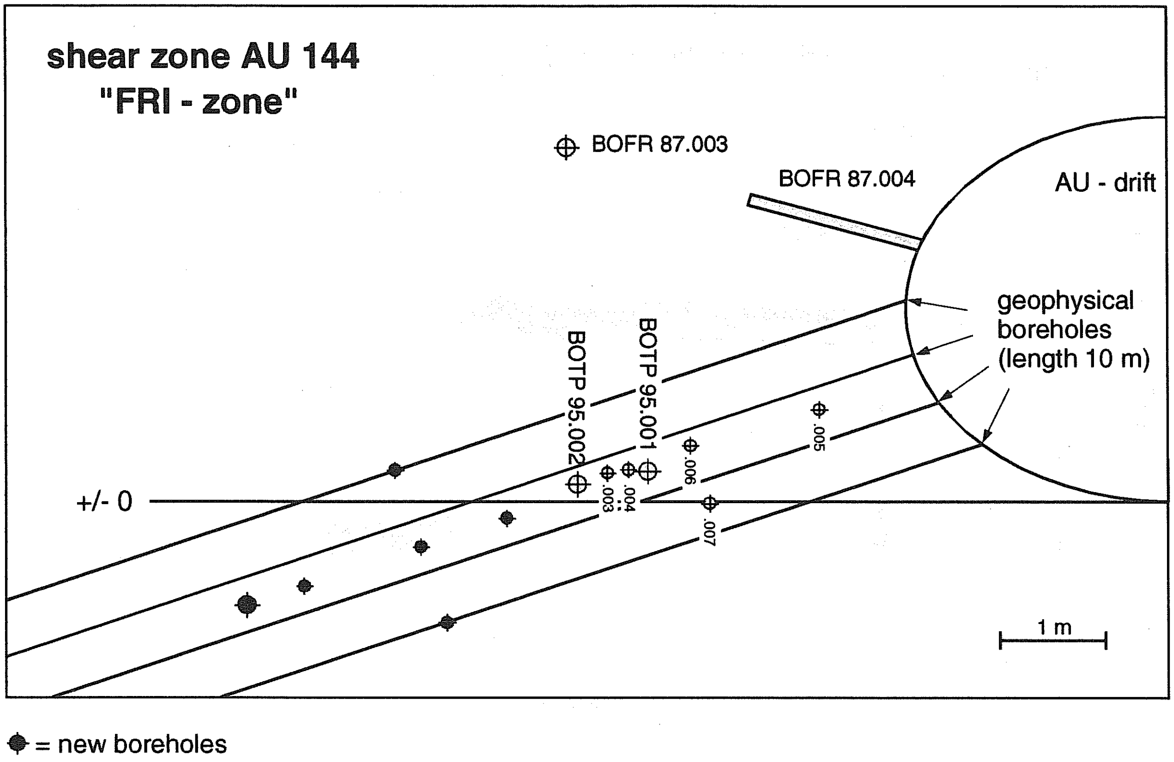

Fig. 1 Location of the boreholes intersecting the FRI zone at the GTS

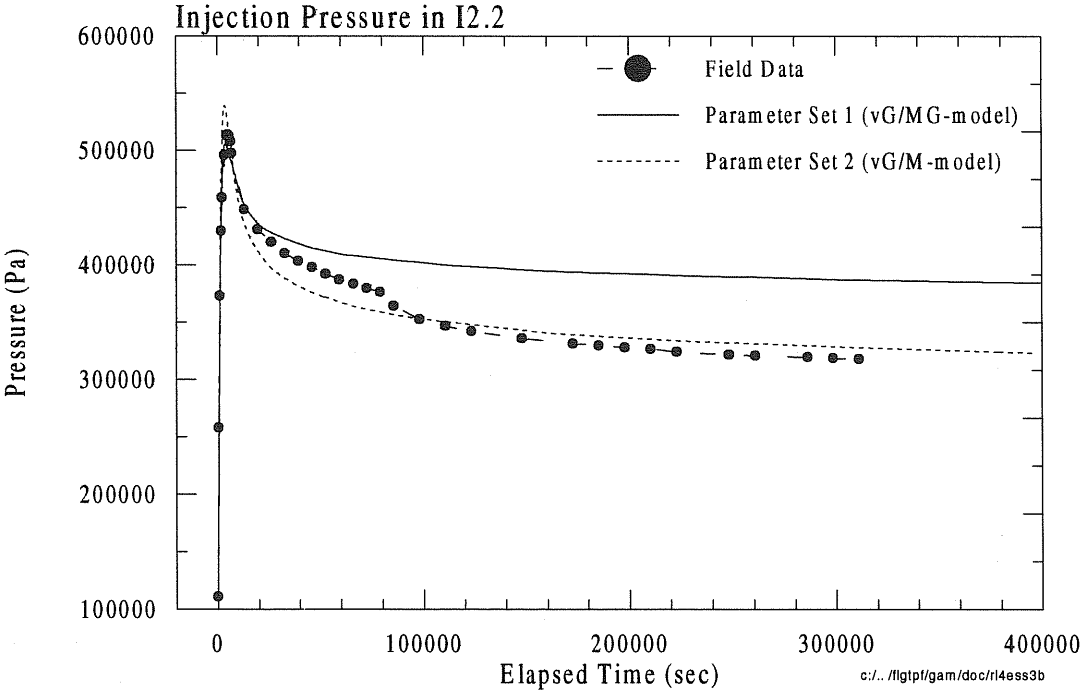

Fig. 2 Injection pressure response for establishing the two-phase dipole flow field

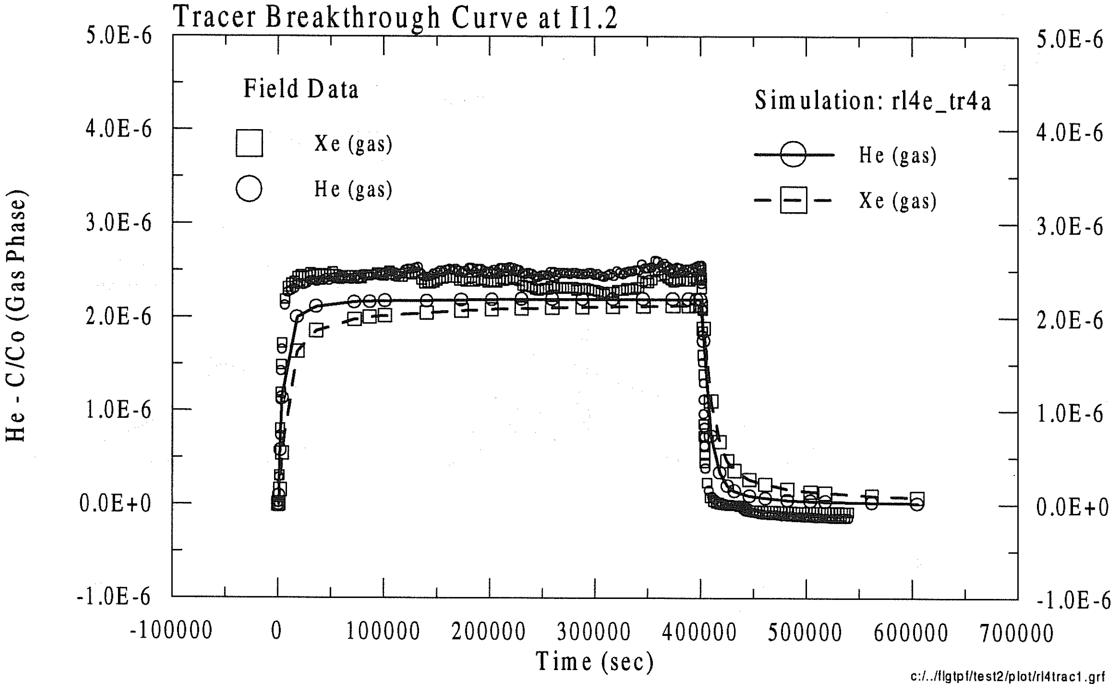

Fig. 3 Gas tracer breakthrough at test interval I1.2 from field experiment and numerical simulations.

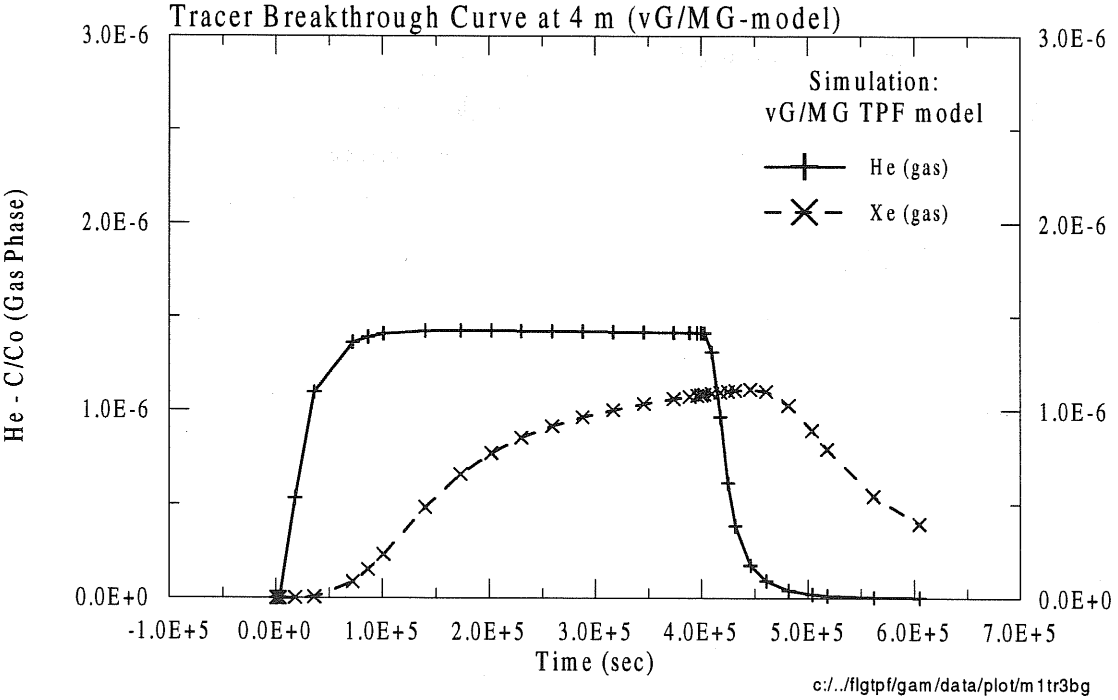

Fig. 4 Simulated tracer breakthrough curves (gas phase) in the planned extraction interval at 4 m.