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Äspö Hard Rock Laboratory

Äspö Task Force on Modelling of Grounwater Flow and Transport of Solutes

Proceedings from the 13th task force meeting at Carlsbad, NM, USA, February 8-11, 2000

Part 1 of 2: Description and Task 4 contributions

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May 2000

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Mansueto Morosini (ed.)
Svensk Kärnbränslehantering AB

June 2000

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1 Introduction

The Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes is a forum for the organizations supporting the Äspö HRL Project to interact in the area of conceptual and numerical modelling of groundwater flow and solute transport in fractured rock. In particular, the Task Force proposes, reviews, evaluates and contributes to such work in the Project.

The work within the Äspö Task Force constitutes an important part of the international co-operation within the Äspö Hard Rock Laboratory. The group was initiated by SKB in 1992 and is a forum for the organisations to interact in the area of conceptual and numerical modelling of groundwater flow and transport. The work within the Task Force is being performed on well-defined and focused Modelling Tasks and the following have been defined so far:

- **Task No 1**: The LPT-2 pumping and tracer experiments. Site scale.
- **Task No 2:** Scoping calculations for a number of planned experiments at the Äspö site. Detailed scale.
- **Task No 3:** The hydraulic impact of the Äspö tunnel excavation. Site scale.
- **Task No 4:** TRUE - The Tracer Retention and Understanding Experiment, 1st stage. Non-reactive and reactive tracer tests. Detailed scale.
- **Task No 5:** Impact of the tunnel construction on the groundwater system at Äspö, a hydrological-hydrochemical model assessment exercise.

Presently eight foreign organizations in addition to SKB are participating in the Äspö HRL. Together these organisations involve twelve modelling groups.

The participating organizations are: Japan Nuclear Cycle Corporation (JNC), Japan; Central Research Institute of Electric Power Industry (CRIEPI), Japan; Agence National Pour la Gestion des Déchets Radioactifs (ANDRA), France; Posiva Oy, Finland; Nationale Genossenschaft für die Lagerung von radioaktiver Abfälle (NAGRA), Switzerland; Bundesministerium für Bildung, Wissenschaft, Forschung und Technologie (BMWi), Germany , Empresa Nacional de Residuos Radiactivos (ENRESA), Spain and US DOE/Sandia National Laboratories, USA.

2 Scope

This report summarises the main findings of the modelling work done in the Task Force since the previous meeting and presented at the 13th Task Force meeting held 7-11 February, 2000 at Carlsbad, NM, USA. The report also constitutes a status report of the Task Force work. Task 1-3 has been completed and the subject of this report is the modelling performed in Task 4 and Task 5.

Specifically, these proceedings include the modelling results of Task 4F from the different modelling groups compiled into common tables and graphs for the purpose of comparison. For Task 5 the first predictive modelling results on the groundwater flow and mixing proportions of different water types are presented in interim reports or slides from the oral presentations.

Contributions for Tasks 4F and 5 were received during the meeting from the modelling groups according to Table 2-1.

Table 2-1. Modelling contributions.

Modelling Group	Task 4F Evaluation of STT2	Task 5 Modelling 2900-3600m + evaluation
ANDRA/ANTEA	n/a	presented
ANDRA/CEA	n/a	presented
ANDRA/ITASCA	n/a	presented
BMWi/BGR	presented	presented
CRIEPI	presented	presented
DOE/SANDIA	presented	n/a
ENRESA/ULC	n/a	presented
JNC/GOLDER	presented	presented
NAGRA/PSI	presented	n/a
POSIVA/VTT	presented	presented
SKB/WRE	presented	n/a
SKB/ChE	presented	n/a
SKB/CFE	n/a	presented
SKB/INTERA	n/a	presented

n/a : not applicable

Reports produced within the framework of the Äspö Task Force published since the previous 12th Task Force meeting are listed in the reference list.

3 Task 4 – Tracer retention and understanding experiments, 1st stage.

3.1 Background

Within the Äspö HRL project, a programme called Tracer Retention Understanding Experiments (TRUE) has been defined for tracer tests at different experimental scales. The overall objective of the TRUE experiments is to increase the understanding of the processes which govern retention of radionuclides transported in crystalline rock, and to increase the credibility in computer models for radionuclide transport which will be used in the licensing of a repository.

The first tracer test cycle (TRUE-1) constitutes a training and testing exercise for tracer test technology on a detailed scale using non-reactive and reactive tracers in a simple test geometry. In addition, supporting technology development is performed in order to understand tracer transport through detailed aperture distributions obtained from resin injection. The TRUE-1 test cycle is expected to contribute data and experience that will constitute the necessary platform for subsequent, more elaborate experiments within TRUE.

3.2 Overview of TRUE-1 tracer test experiments

The Modelling Task 4 consist of several modelling exercises in support of the TRUE-1 tracer tests including predictive modelling where the experimental results are not available beforehand. Previous modelling task, that are now completed are:

- Task 4A consisted of modelling in support of the development of the descriptive structural model of the test site.
- Task 4B whose scope of was to perform modelling in support of the experimental design.
- Tasks 4C and 4D were defined to perform predictive modelling of non-sorbing tracer tests at the TRUE-1 site, including a comparison of model outputs with experimental results.

All these tasks were to a great extent preparatory steps for Tasks 4E and 4F that comprise predictive modelling of tracer tests performed with collection of sorbing, slightly sorbing and non-sorbing tracers. These tests were performed between packed off boreholes penetrating a water-conducting geological feature with a "simple" structure, Feature A. The tracer tests were preceded by a characterisation of the site and a preliminary tracer experiment.

A bibliography of modelling results performed for Task 4 is compiled in Appendix

Task 4E and 4F

Task 4E and 4F are based on data from sorbing tracer tests. The objectives of the sorbing tracer test part of TRUE-1 /Andersson et al, 1997B/ are:

- Test equipment and methodology for performing tracer tests with weakly sorbing radioactive tracers
- Increase understanding of transport of tracers subject to sorption in the studied feature
- Obtain parameters which describe retention of tracer transport
- Test different weakly and moderately sorbing radioactive tracers

The overall experimental scope includes:

- Two main geometrical configurations KXTT4:R3□KXTT3:R2 and KXTT1:R2 □ KXTT3:R2
- 2 pump rates
- Weakly (Na, Ca, Sr) and moderately (Rb, Cs, Ba) sorbing tracers as well as the two non-sorbing tracers tritiated water and uranine.
- STT-1 (q=400 ml/min): highest flow rate, diffusion into the matrix (dead end pores are minimised). Flowpath was KXTT4:R3□KXTT3:R2.
- STT-1b: A complementary injection of sorbing tracers in KXTT1:R2 (q=400 ml/min)
- STT-2 (q=200 ml/min): intermediate flow rate, surface sorption, however there are questions regarding the effect of diffusion into the rock matrix. Flowpath was KXTT4:R3□KXTT3:R2.

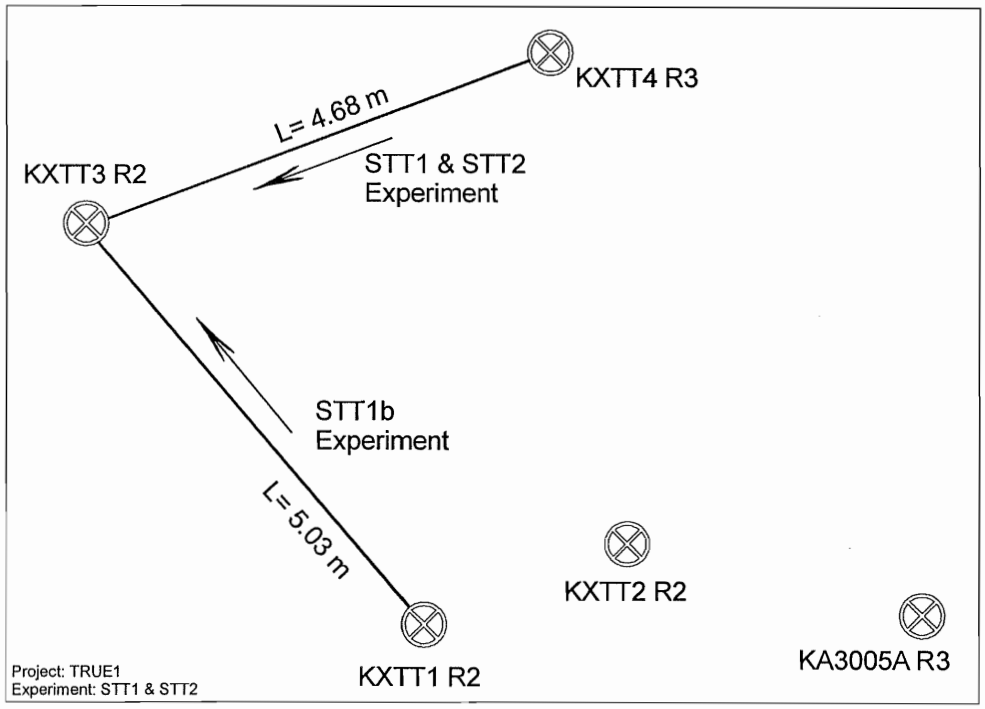


Figure 3-1 Borehole intersections with Feature A shown in the plane of the feature. Distances given in metres.

3.3 Modelling results Task 4F

The modelling work aimed at resolving issues of methodology, transport geometry, processes and to assess uncertainties. These issues were addressed to various degrees by the modelling groups. The deconvolution of STT-2 data (Elert and Svensson, Appendix A) which was commissioned previously, reported that the two peaks in the response are probably due to geometry rather than on methodology, since these peaks were reproduced in spite of the deconvolution approach. The deconvolution method proved successful for all tracers in STT-2 and in discriminating between source term and transport processes.

An assessment supporting the potential of deconvolution was presented (P. Marschall, Appendix A) and suggestions made on ways to improve the method.

The conclusions of some of the modelling groups drawn from the performed evaluation of the modelling of STT-2 is summarised below.

BGR

- It is necessary and very important to determine the fracture geometry and hydraulic patterns under the test conditions. The latter can be determined by iterative modelling of flow and transport.

- Flow and transport parameter values can be determined by numerical modelling of hydraulic and transport tests.

- Sorption and decay properties of radioactive tracers can be modelled numerically.

- Groundwater flow and transport of solutes in the fractured rock can be simulated using the Rockflow program.

Sandia

- The general shape and timing of STT-2 breakthrough curves is predicted by the blind prediction

- A single-path multirate model provides good fits to the tail of the breakthrough curves, but is unable to account for the two-path advective behaviour.

- The flow parameters are significantly different from the Sandia analysed STT-1 estimates

- The transport parameters also differ from the Sandia analysed STT1 estimates.

Golder

The modelling carried out for Task 4F2 was not very useful, since nothing was learnt about the nature of flow and transport properties. Rather, what was learned is the limitations of model calibration, and the number of variables which are available to match the observed breakthrough curves. The prediction was calibrated to the level possible without detailed understanding. Because the forward model is confined to physical parameters and structures, there are limited degrees of freedom for model calibration and improvement. In order to improve the geochemical model fit, for example, it was necessary to add structural features to the model that had not been characterised by SKB.

WRE

- A calibration factor f=40 was needed in order to explain the experiment.

- Feature A characterised by rim zone with properties likely to be different compared to MIDS.

- The enhaced mass transfer is attributed to increased porosity in the rim zone, increased K_d^m of matrix and increased flow wetted surface.

KAT

No good predictions were made of the sorbing tracer tests. The predicted breakthrough times were shorter. The actual longer breakthrough times could be explained by various

processes: larger diffusion/sorption, sorption of gouge/filling, flowrate is smaller than average, and diffusion into stagnant water.

PSI

A very simple flow and transport model based on the double porosity streamtube concept (DPM) was used which provided fairly good predictions for all three tracer tests. However, the input from the geologists (and other scientists) was needed for an appropriate model structure. The DPM-model accounts for the most important transport mechanisms. It is a simple but versatile and "understandable" model with few (lumped) transport parameters (no fudge-factors) and no further transport mechanism was needed.

3.4 Performance of tracer test (RC4) with new injection equipment

A new radially converging tracer test with conservative tracers was completed with the following objectives:

- to test a new down-hole equipment in-situ under ambient flow and pressure conditions
- to demonstrate that a well-defined tracer pulse injection can be performed
- to characterise a new flow path in Feature A

The RC-4 transport geometry involved KXTT3 R2, as injection section, with withdrawal from KXTT4 R3 and KXTT5 P2, see Appendix A.

Four tracer injection were performed according to Table 3-1. The injection and breakthrough curves are presented in Appendix A.

Table 3-1 Injection and recovery performance of the RC4 experiment.

Inject #	Bh Section	Tracer	Max Conc (ppm)	Initial rate (mL/h)	Exchange efficiency (%)	Sampling time (h)	Recovery (%)
1	KXTT4 R3	AminoG	750	46	97	140	85
2	KXTT5 P2	Uranine	630	18	98	50	0
3	KXTT4 R3	AminoG Acid	700	300	0	95	>60
4	KXTT5 P2	Rhodamine WT	700	21	99.0	95	>50

From this experiment it was concluded that the new borehole equipment in combination with a longer exchange period has significantly improved the tracer pulse injection procedure (99.9% reduction of tracer mass). Furthermore, a new flow path, KXTT5 P2 - KXTT3 R2 has been tested in Feature A and found to be connected but more difficult to control. Finally, additional transport data for the flow path KXTT4 R3 - KXTT3 R2 has been produced for two new sink strengths. A compilation of Task 4 presentations given at the meeting is provided in Appendix A.

3.5 Complementary laboratory data (TRUE-1)

Rock samples from the TRUE-1 borehole cores were subjected to detailed analysis in the laboratory with the objectives to obtain

- Detailed porosity and diffusivity measurements of Feature A mylonite and altered diorite from KXTT2.
- Penetration profile of KXTT1 sample, exposed to through diffusion experiment for 3 years.
- Porosity homogeneity and distribution studies using ^{14}C-labelled MMA impregnation on Feature A intercept in core from KXTT3.

It was found that the water saturation porosity of material from KXTT2 varied from 0.33% and 0.97 %. When modelling performed through diffusion data, best fit with the experimental data was obtained when keeping the porosity fixed and allowing for a distribution of diffusivity (mean D_e and σ_{De}). The MMA impregnation studies indicate decreasing porosity from the fracture surface and into the rock. The results indicate porosities > 2.5% in the immediate vicinity of the fracture surface constituting the intercept with Feature A in KXTT3.

Some of the results from these studies were presented at the meeting are given in Appendix A (J. Byegård).

4 Task 5 – Integration of hydrochemistry and hydrogeology.

4.1 Background

The chemical composition of the groundwater is a result of the interaction with the rock minerals and the groundwater. The degree of interaction is a function of groundwater transport and residence time. It is therefore of interest to study the combined hydrodynamic and hydrochemical evolution of a groundwater system. However, major difficulties are recognised because the present day (and past) hydrodynamic conditions have resulted in groundwater mixing to varying degree.

The fifth modelling task of the Äpö Task Force, Task No 5, is a hydrological-hydrochemical model assessment exercise that specifically studies the impact of the tunnel construction on the groundwater system at Äspö. The task definition has been successively refined resulting in the following major objectives:

- Assess the consistency of groundwater flow models and hydrochemical mixing-reaction models through integration and comparison of hydraulic and chemical data obtained before and during tunnel construction.
- Develop a procedure for integrating hydrological and hydrochemical information that could be used in the assessment of potential disposal sites.

Organisations participating in this modelling task are SKB, ANDRA, POSIVA, BMWi, JNC, CRIEPI and ENRESA.

The modelling is performed with the objective to replicate observed groundwater compositions and flow in the tunnel and at a few control points away from the tunnel. The framework to support this modelling effort consisted of data packages delivered to the modellers at different time intervals (see Appendix C).

4.2 Modelling results, 2900-3600m

The main modelling purpose at this stage was to predict the of flow pattern, the mixing proportion in terms of reference waters, and the advective travel time distribution at the given control points. The different groups performed the modelling to varying degrees. The modelling results and presentations are compiled in Appendix B. Data delivered by SKB to the modelling groups prior to TF#13, which formed the basis for the modelling, is listed in Appendix C.

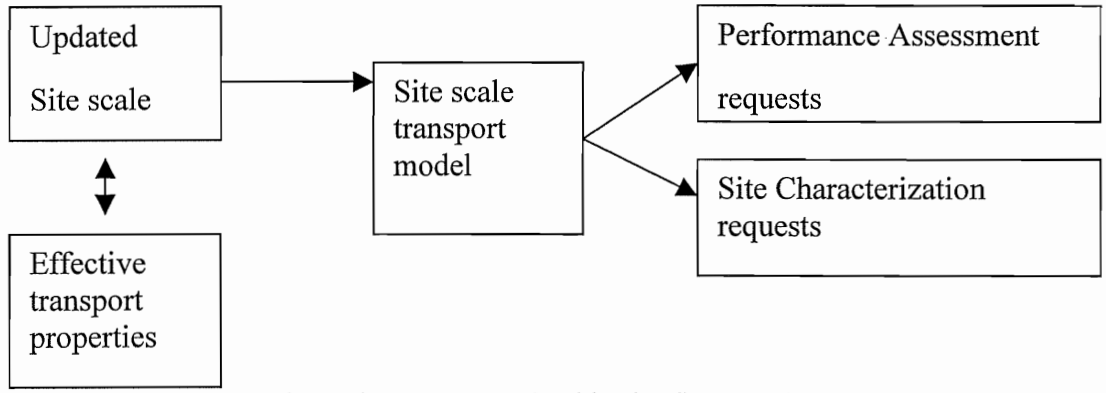
Some general conclusion can be drawn from the modelling results. The level of ambition varies between the modelling groups due to the fact that integration of hydrogeology and hydrochemistry is still at its initial stage of development. Consequently, there are few existing models that successfully integrate the physics and chemistry of the groundwater system and the achieved integration has mainly involved

mixing proportion calculations. Generally, water/rock chemical reactions have not been addressed. The results largely support M3 as a useful tool for mixing proportion calculations; POSIVA's alternative approach is very promising but has still to be fully tested. Although the modelling of the REDOX zone carried out by ENRESA exemplified a successful integration of hydrochemistry and hydrodynamic, unfortunately it is not representative for the Äspö site as a whole.

5 Task 6 – Flow and transport between different scales

A proposal for the Task 6 was discussed during the meeting and at the workshops held in connection to the meeting. It was concluded the mission for Task 6 should be to a) optimise the site characterisation and b) to interact with PA. The following subtasks are proposed, they should interact with each other,

Site characterization	Uncertainty and robustness	Performance assessment
Improve the site scale model	Backtrack evolution of structural models	Introduce PA perspective
Reanalyse LPT-2	Do sensitivity analysis	Relevant measures
	Extrapolate? How?	Model PA problem



The basic components of the task are summarised in the figure below.

The meeting was concluded with a joint summing up of the workshops and Delegates were requested to give a hint on their prospective interest in Task 6.

6 References

S. McKenna, 1999: Solute transport modelling of the Äspö STT1b tracer tests with multiple rates of mass transfer. Äspö Task Force task 4EInternational Progress Report ICR 99-02, SKB Stockholm, Sweden

H. Shao and L. Liedtke, 1999: Modelling the reactive-radioactive and sorbing tracer tests in fractured rock. Äspö Task Force Task 4E and 4F. International Progress Report ICR 99-03, SKB Stockholm, Sweden

M. Morosini, 1999: Proceedings from the 12th Task Force Meeting at Gimo, Sweden, April 20-22, 1999. International Progress Report IPR-99-22, SKB Stockholm, Sweden.

M. Elert and H. Svensson, 1999: Deconvolution of breakthrough curves from TRUE-1 tracer tests (STT-1 and STT-1b) with sorbing tracers. Äspö Task Force Task 4E. IPR-99-35. International Progress Report IPR-99-35, SKB Stockholm, Sweden

Appendix A – Task 4E&F modelling results

- Status of TRUE-1 and conclusions (Anders Winberg, Conterra AB)
- Evaluation of Task 4E&F (Mark Elert, Kemakta)
- Deconvolution of Task 4F breakthrough curves (Mark Elert, Kemakta)
- On the potential of deconvolution (Paul Marschall, NAGRA)
- Resolution of issues and uncertainties in calculations of the transport of radioactive substances (Lutz Liedtke, BGR)
- Numerical analysis with FEGM/FERM for Task 4F (Y. Tanaka, CRIEPI)
- Estimation of STT-2 tracer tests (S. McKenna, Sandia)
- Task 4F2 Modelling (W. Dershowitz, Golder)
- Conclusions from modelling Task 4E&F (A. Jacob, PSI)
- Final evaluation of TRUE-1 tests (J O Selroos, SKB)
- TRUE Task 4E&F channel network model (L. Moreno, KTH-KAT)
- Results from RC-4 tracer experiment (P. Andersson, Geosigma)
- Results of complementary laboratory experiment. (J. Byegård, CTH)

Status of TRUE-1 and conclusions

A Winberg (Conterra AB)

Final Report of The First TRUE Stage
Summary conclusions

Anders Winberg, Conterra AB

Presented at the 13th meeting
SANDIA National Laboratories, Carlsbad, NM
February 8-11, 2000

Final Report of the First TRUE Stage Conclusions - Tracer test methodology

- **Available tracer test methodology has been successfully adapted and applied in the detailed scale at the prevailing conditions (high pressures (P >30 bars) and high salinity ([Cl] > 5000 mg/l)**
  - **Feature A is connected in a transport sense over its investigated area.**
  - **The use of tracer dilution tests in combination with pumping has proven to be a good tool for subsequent tracer test design.**
  - **The existing natural gradient in the investigated Feature A (10 %) controls the background flow and makes it difficult to perform high-recovery tracer tests over longer distances (> 5 m) and at low pump flow rates (< 0.2 l/min).**
  - **Two flow paths in Feature A qualified for tests with radioactive sorbing tracers have been successfully used.**

Final Report of the First TRUE Stage Conclusions - Cationic sorbing tracers

- **The proposed cationic sorbing tracers featured by sorption by cation exchange have been successfully applied in laboratory experiments and in *in situ* experiments.**
  - **The sorbtivity of the exposed geological material is shown to depend on the concentration of biotite.**
  - **The sorption in the batch laboratory experiments is observed to be time dependent, ie. the evaluated K_d increase with increasing contact time.**
  - **Breakthrough in the *in situ* experiments has been observed for the sorbing tracers Na^+, Ca^{2+}, Sr^{2+}, Rb^+, Ba^{2+}, Cs^+, K^+, Co^{2+}. Uranine, tritiated water (HTO), $^{131}I^-$ and $^{82}Br^-$ were used as conservative tracers.**
  - **The sorbtivity of the tracers used in the laboratory experiments on geological material from Äspö, show the following relative order; $Na^+ < Ca^{2+} \approx Sr^{2+} < <Rb^+ \approx Ba^{2+} < Cs^+$. The observed relationship is also consistently observed in the *in situ* test results.**

Final Report of the First TRUE Stage Conclusions - Evaluation framework

- **The developed Lagrangian evaluation framework has been demonstrated to be applicable for modelling the dominant effects of reactive transport in a single fracture.**
  - A key result is the the parameter β which integrates the inverse velocity-weighted aperture along the flow path. It controls surface sorption and diffusion/sorption into the matrix. A linear relationship $\beta = k \cdot \tau$ was found suitable for modelling retention in Feature A ($k_0 \approx 3400$ m^{-1})
  - Unlimited diffusion/sorption in the rock matrix is the dominant retention mechanism in Feature A over the time scales of the TRUE-1 *in situ* experiments. The effects of equilibrium surface sorption and limited sorption in gouge material on tracer retention are observable, but second order. Similarly the effects of diffusion into stagnant water zones is small.
  - Assuming a strict linear relation between β and τ, the proportionality factor k is equivalent to the "flow wetted surface" per volume of water" (a_w). The value k is within bounds of a_w reported in the literature.

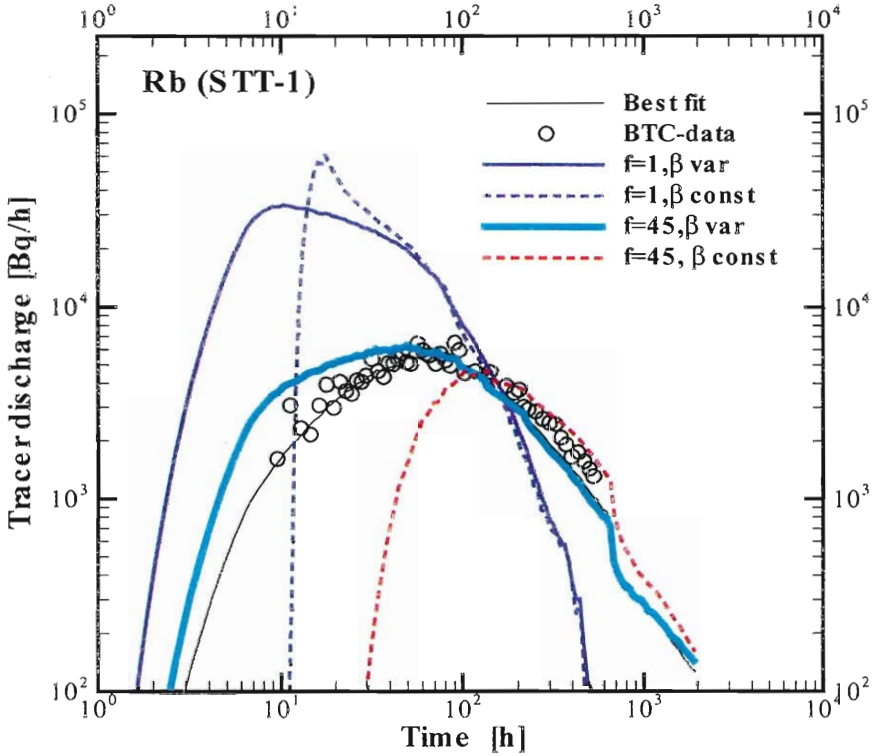
Final Report of the First TRUE Stage Conclusions - Parameters for the main retention processes

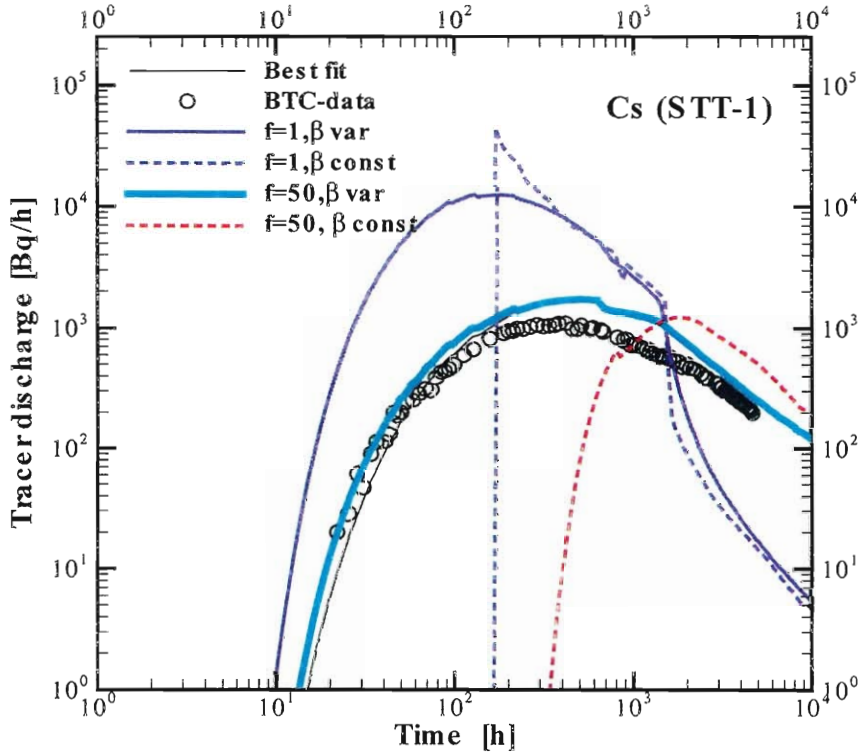
- **Values of parameters for the main retention processes included in evaluation concept (LaSAR) have been obtained either from laboratory data, or through estimation using *in situ* data and the calibrated parameter group which controls diffusion/sorption in the matrix rock.**
  - **The parameter values for diffusion/sorption estimated for *in situ* conditions have been shown to be enhanced compared to those measured in the laboratory (f = 32-50). The enhancement is mainly attributed to higher values on matrix porosity and/or diffusivity applicable to *in situ* conditions compared to values measured in the laboratory. A minor contribution attributed to the flow-dependent parameter *k*.**
  - **The parameters related to sorption in gouge material have been calibrated using *in situ* breakthrough data. Effects of sorption in gouge material have been found to be most evident for the weakly sorbing tracers Na and Sr, since for these tracers, matrix diffusion/sorption is relatively small.**

Final Report of the First TRUE Stage Conclusions - Predictive capability

- The use of laboratory data on diffusion/sorption parameters constitutes a basis for robust and relatively accurate predictions of reactive tracer breakthrough, in particular of first arrival.
  - This provided that the water residence time distribution (conservative breakthrough) is known (can be assessed) and that variability in the β parameter is accounted for.

Predictive capability and effect of variability in β exemplified using a) Rb and b) Cs breakthrough in the STT-1 test. Only matrix diffusion/sorption and surface sorption are considered except in the "best fit" curve where sorption in gouge is added





Final Report of the First TRUE Stage Conclusions - Altered rim zone

- **The altered rim zone along the studied feature is interpreted to show enhanced, albeit variable, porosity/diffusivity in relation to the unaltered matrix rock, and is important for the tracer retention over the time scales of the TRUE-1 experiments.**
  - **The rim zone is interpreted to be made up of primarily of altered Äspö diorite and mylonite, the latter with a lower porosity/diffusivity.**
  - **The average range of porosity in the rim zone of Feature A is estimated to be 2-2.4 %**
  - **Using the assumed range of *in situ* porosity of the rim zone and the calibrated parameter group defining diffusion/sorption in matrix rock, estimates of *in situ* values of important transport parameters have been made.**

Final Report of the First TRUE Stage Conclusions - Pore space/aperture data

- **A workable technology and procedure for obtaining pore space/aperture data from *in situ* epoxy resin injection and subsequent excavation and analysis has been developed and applied in a Pilot Resin Injection Experiment (at a different location than the TRUE-1 experiment).**
  - **A fracture system with a one order of magnitude lower transmissivity than Feature A has been subject to resin injection.**
  - **The average aperture of the analysed samples are 240 and 270 μm, respectively with a coefficient of variation of about 40 %.**
  - **Evaluated variograms of the aperture mapped by the epoxy indicate practical ranges varying between 0.003 to 0.005 m.**

Final Report of the First TRUE Stage Conclusions - Site characterisation

- **The performed characterisation provides a powerful set of tools for assessment of conductive geometry and connectivity in future preliminary site characterisation, and in particular during future detailed site characterisation.**

  - ✎ **The use of borehole TV imaging in combination with detailed flow logging identifies the conductive features in a borehole.**
  - ✎ **Cross-hole pressure interfere testing, including observations during drilling of a new borehole, provide information on how the conductive features connect.**
  - – **The tracer test methodology developed and used in this work is applicable to characterisation work in various phases of repository development.**

Final Report of the First TRUE Stage Conclusions - Extrapolation

- The performed transport experiments in the laboratory combined with detailed mineralogical and geochemical characterisation provide a platform for export of estimated *in situ* values of transport parameters and generic transport characteristics to a sites with similar geological and chemical conditions.

Final Report of the First TRUE Stage Conclusions - Äspö Task Force

- The close interaction with the Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes has provided important support in initial experimental design. Further, by performing blind model predictions, a basis for a scientific test of our understanding and predictive capability is obtained. The ongoing evaluation of the predictions of tests with sorbing tracers will provide further insight in our understanding of flow and retention in a single feature.

Evaluation of Task 4E&F

M Elert (Kemakta)

Evaluation of modelling of STT-1, STT-1b & STT-2 tests Tasks 4E and 4F

Äspö Task Force meeting 8-11 February 2000

Mark Elert

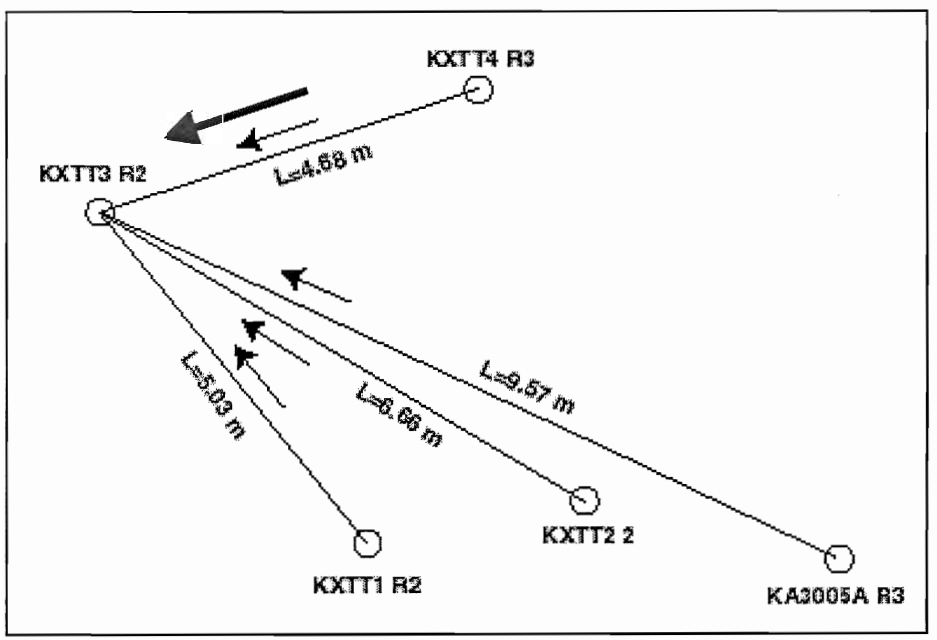
Kemakta Konsult

Introduction

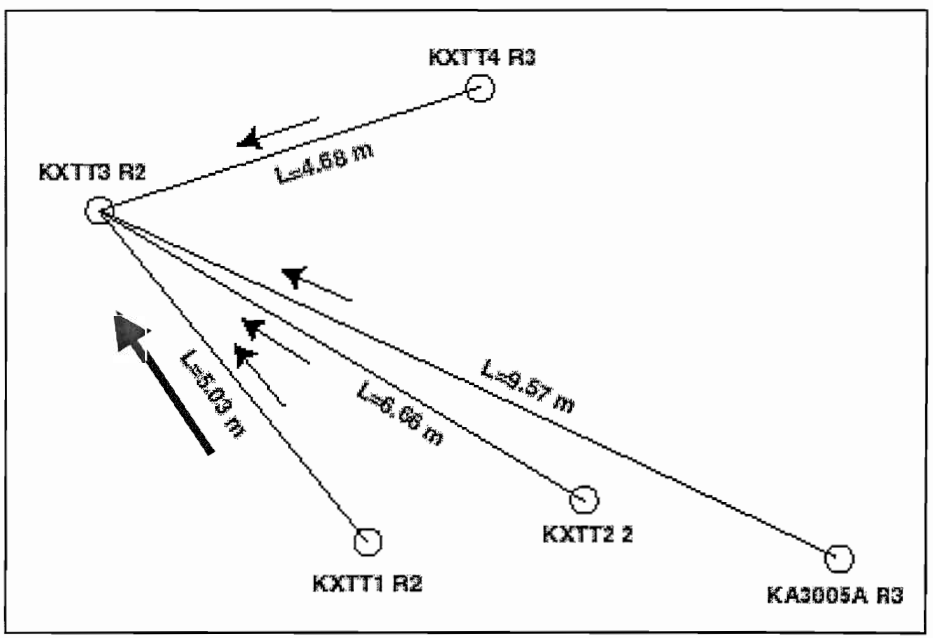
- The evaluation work is ongoing. Waiting for material from modelling groups. So far using:
  - Task Force Meeting Reports (Prediction and experiment evaluation)
  - Modelling Questionnaires
- Preliminary contents of evaluation report:
  1. Introduction
  2. Purpose and set up of experiment
  3. Modelling approaches
  4. Results
  5. Discussion
  6. Conclusions

Experiments

STT-1 (Q=0.4 l/min) & STT-2 (Q=0.2 l/min)



STT-1b (Q=0.4 l/min)



- Non-sorbing, weakly sorbing and moderately sorbing tracers

Modelling approaches

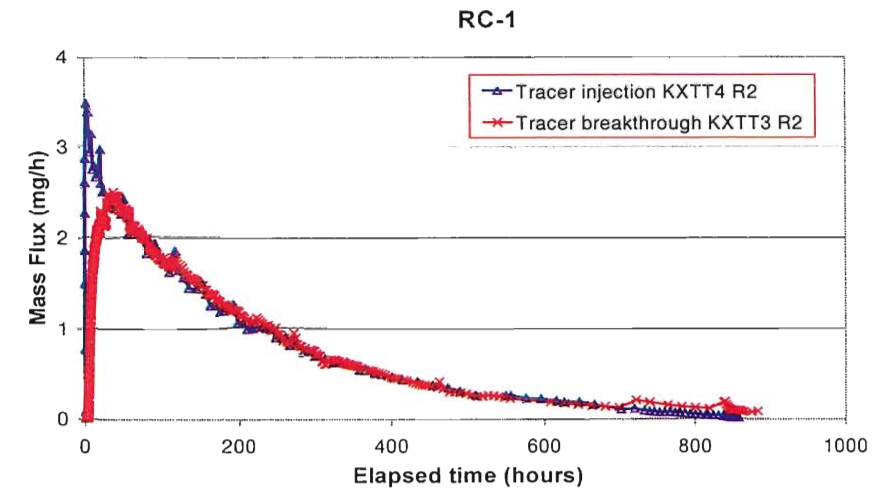
- Types of models
  - Deterministic continuum model (homogeneous/ heterogeneous)
  - Stochastic continuum
  - Deterministic multirate mass transfer model
  - Discrete Fracture Network
  - Channel Network
- Model geometry
  - Most groups considered Feature A as an isolated feature
  - JNC/Golder: Discrete Fracture Network
  - BMWi/BGR: Included Feature B (although with little effect)
  - SKB/KTH-ChE: Channel Network including effect of tunnel
- Processes
  - Darcy flow (head gradients - transmissivity/hydraulic conductivity)
  - Advection
  - Dispersion (presence of different flow paths/ dispersion coefficient)
  - Surface sorption
  - Matrix diffusion and sorption
  - Diffusion into fault gouge
  - Diffusion into stagnant zones

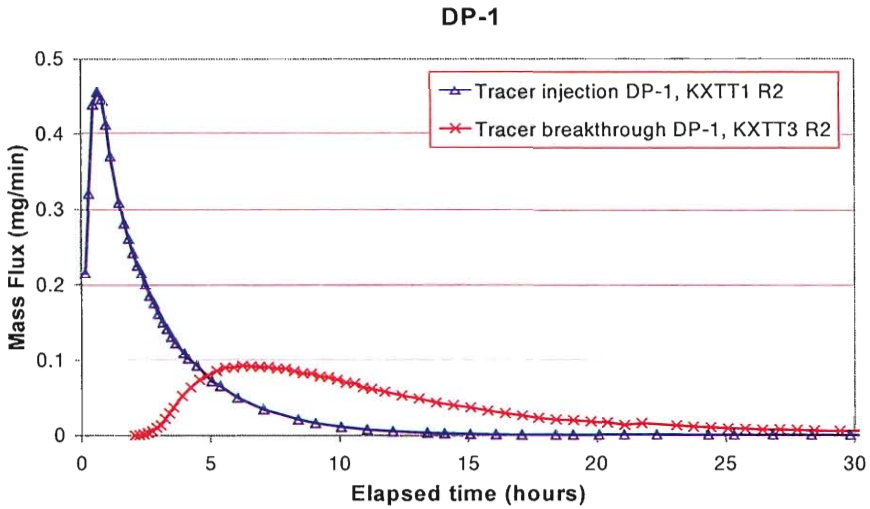
Summary of measured and evaluated parameters for the flow path KXTT4 R3 → KXTT3 R2

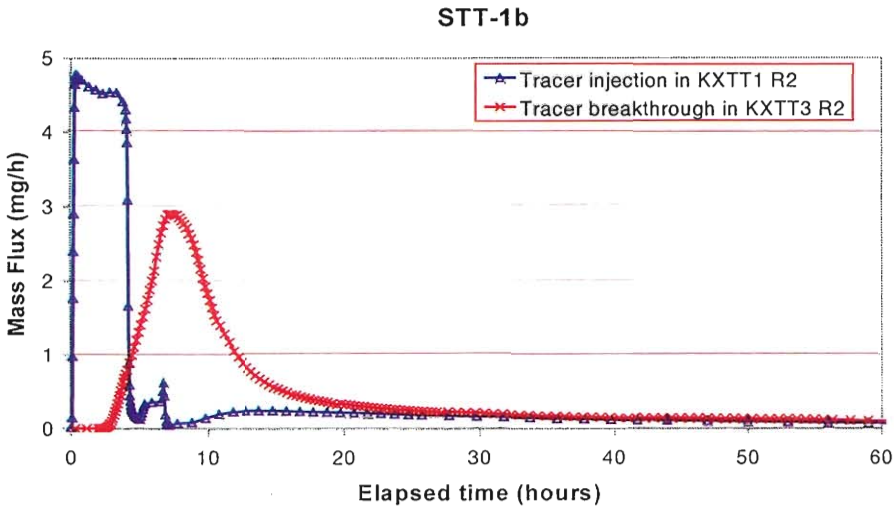
Test*	Q (l/min)	Δh (m)	R (%)	D/v (m)	K_{fr} (m/s)	b (m)	θ_k
RC-1	0.2 (0.4)*	2.8 (6.9)*	100	1.6	$7.1 \cdot 10^{-4}$	$1.4 \cdot 10^{-3}$	$0.5 \cdot 10^{-3}$
DP-5	0.1	3.0	28	0.34	$2.0 \cdot 10^{-4}$	$1.6 \cdot 10^{-3}$	$0.5 \cdot 10^{-3}$
DP-6	0.2	3.6	70	0.48	$4.1 \cdot 10^{-4}$	$2.4 \cdot 10^{-3}$	$0.4 \cdot 10^{-3}$
PDT-1	0.1	1.0	74	0.6	$6.4 \cdot 10^{-4}$	$2.1 \cdot 10^{-3}$	$0.5 \cdot 10^{-3}$
PDT-2	0.2	2.3	99	1.1	$5.9 \cdot 10^{-4}$	$2.0 \cdot 10^{-3}$	$0.6 \cdot 10^{-3}$
PDT-3	0.4	6.8	95	1.7	$4.8 \cdot 10^{-4}$	$1.7 \cdot 10^{-3}$	$0.7 \cdot 10^{-3}$
STT-1	0.4	7.2-10.5	100	2.0	$4.2 \cdot 10^{-4}$	$1.4 \cdot 10^{-3}$	$0.8 \cdot 10^{-3}$
STT-2	0.2	6.1	96	0.35**	$3.4 \cdot 10^{-4}$**	$1.3 \cdot 10^{-3}$**	$1.1 \cdot 10^{-3}$**
				0.46***	$1.0 \cdot 10^{-4}$***	$4.5 \cdot 10^{-3}$***	$4.0 \cdot 10^{-3}$***

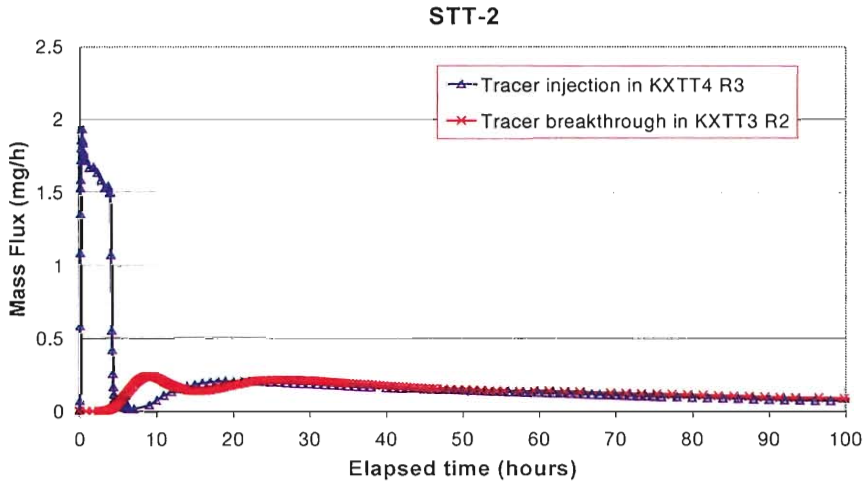
* Pumping increased during experiment
** Flow path #1
*** Flow path #2

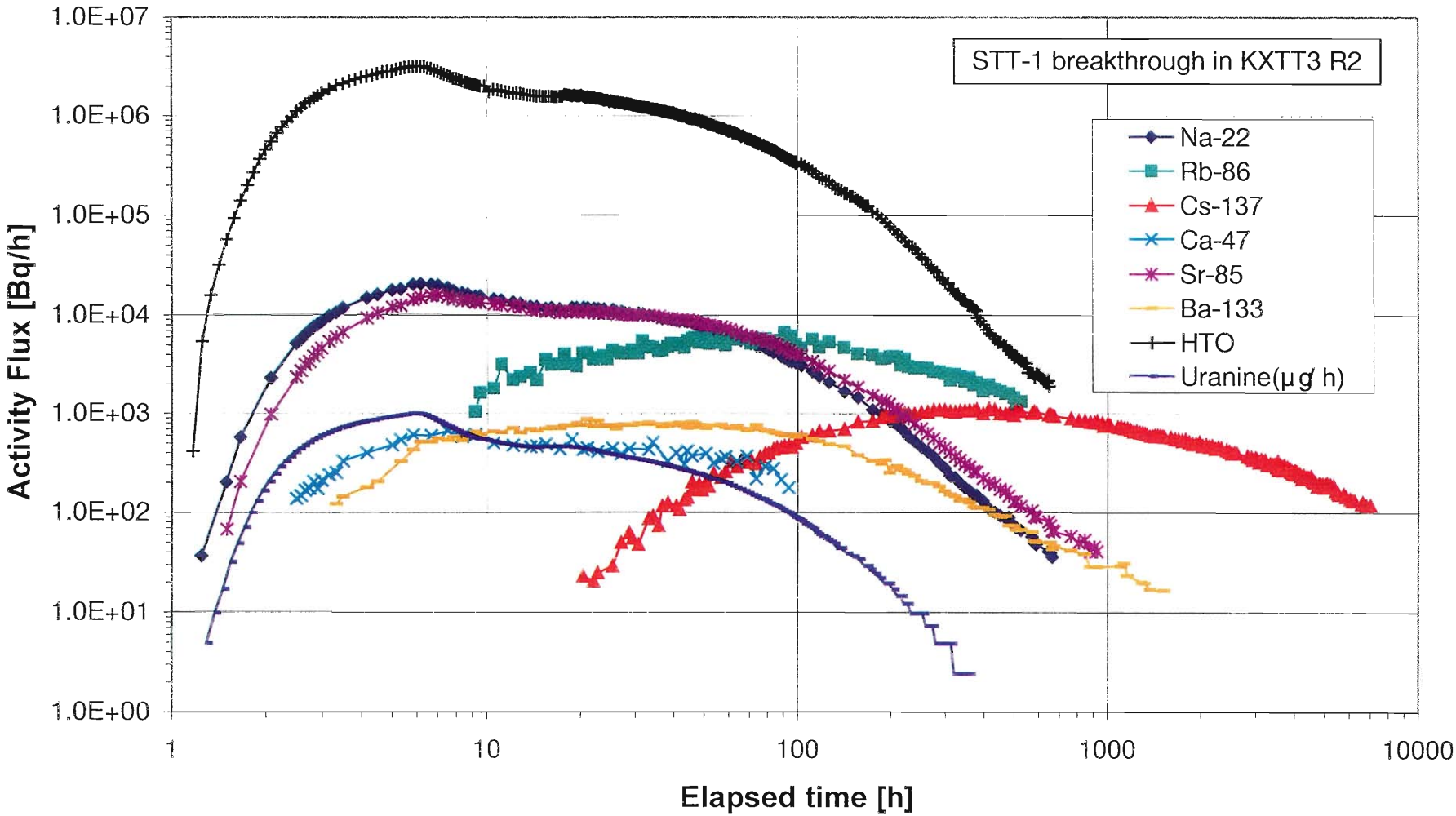
Injection and breakthrough curves



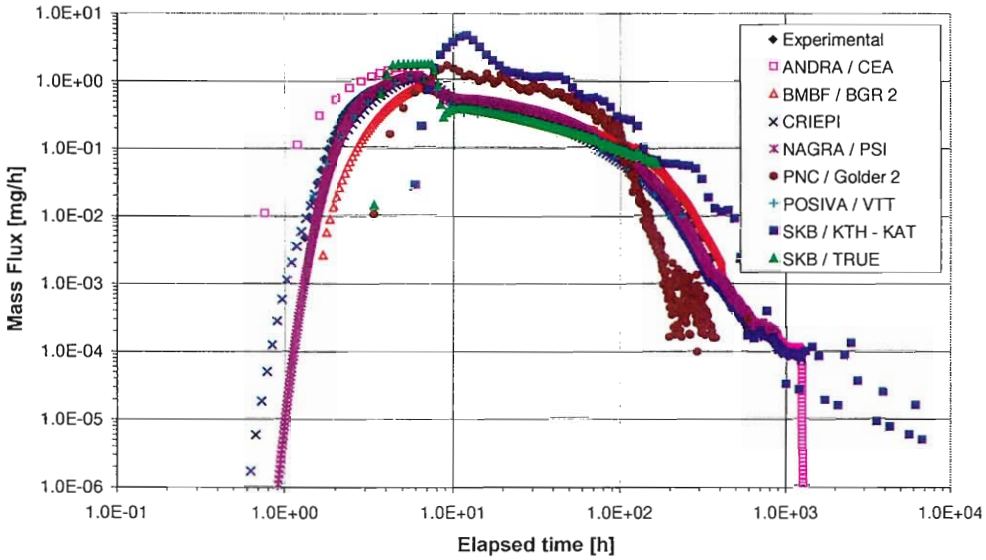


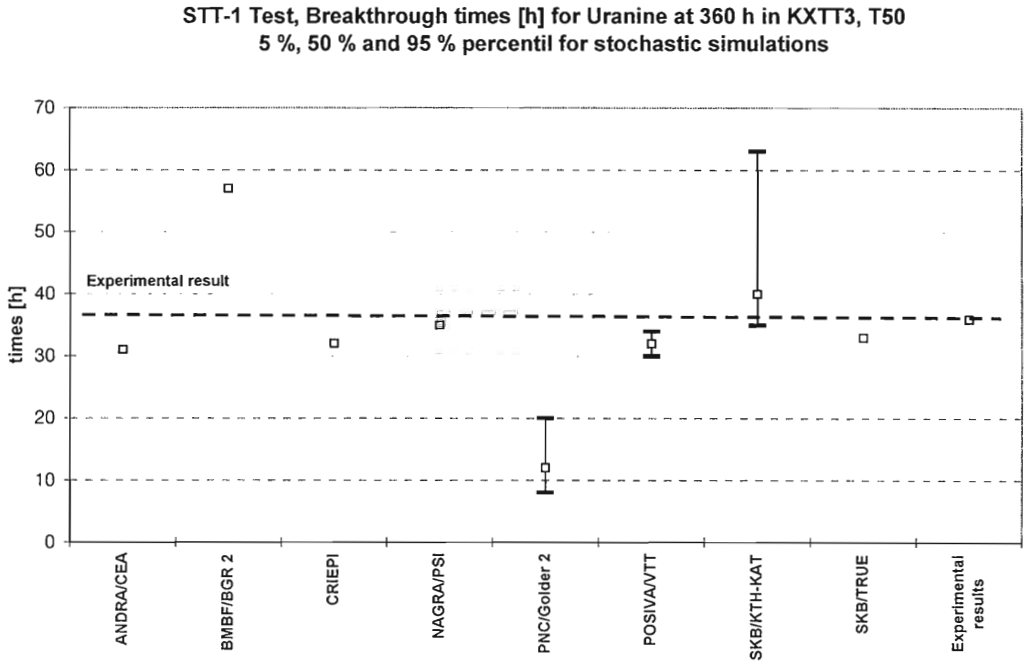





STT-1 breakthrough in KXTT3 R2
Na-22
Rb-86
Cs-137
Ca-47
Sr-85
Ba-133
HTO
Uranine(µg/h)
Activity Flux [Bq/h]
1.0E+07
1.0E+06
1.0E+05
1.0E+04
1.0E+03
1.0E+02
1.0E+01
1.0E+00
1
10
100
1000
10000
Elapsed time [h]

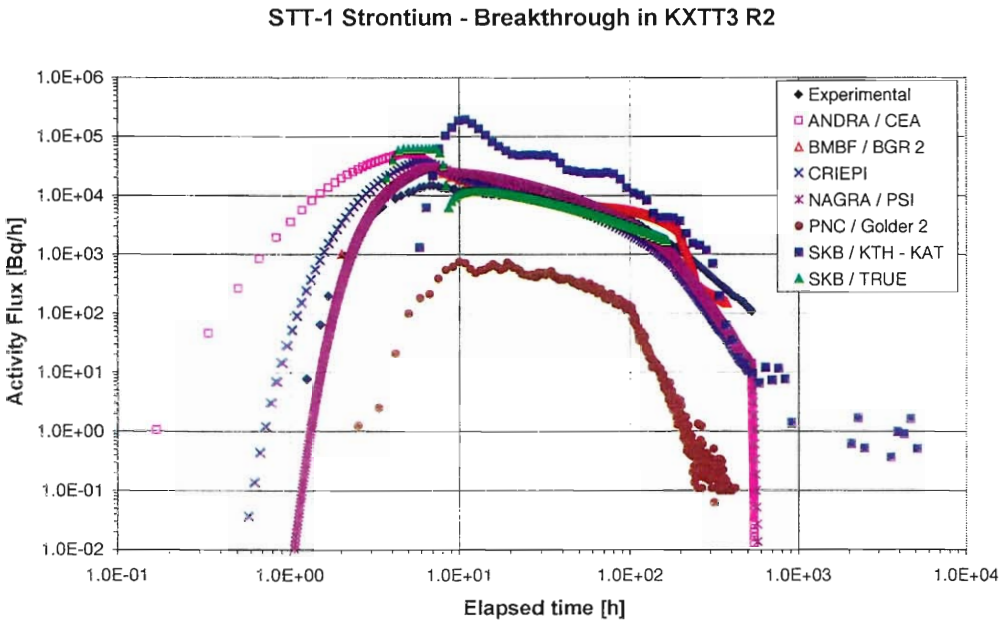
Predictions Uranine STT-1

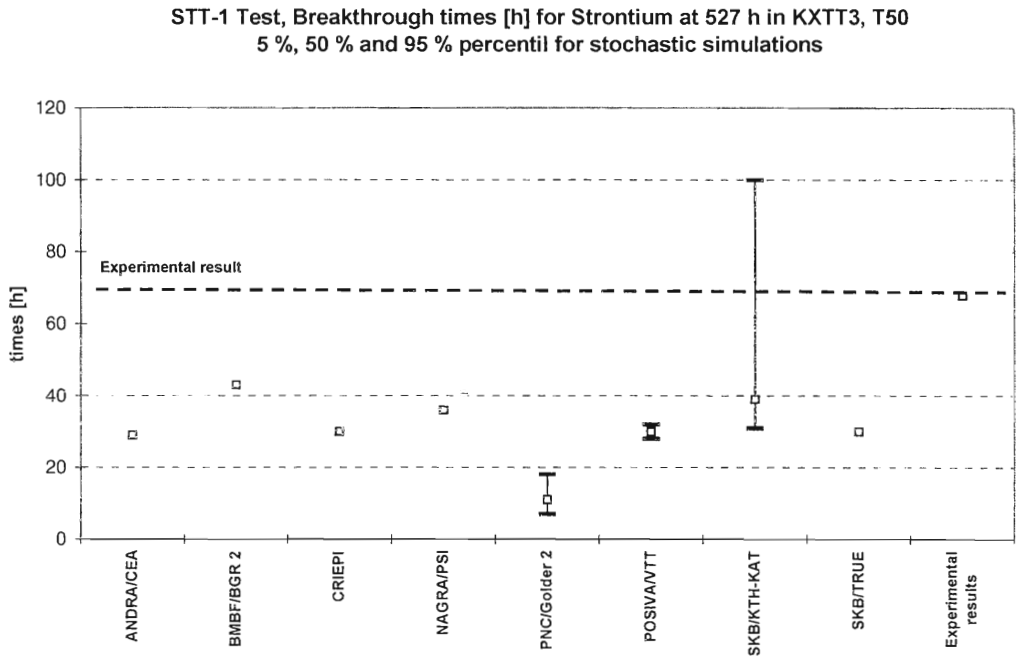




Kemakta

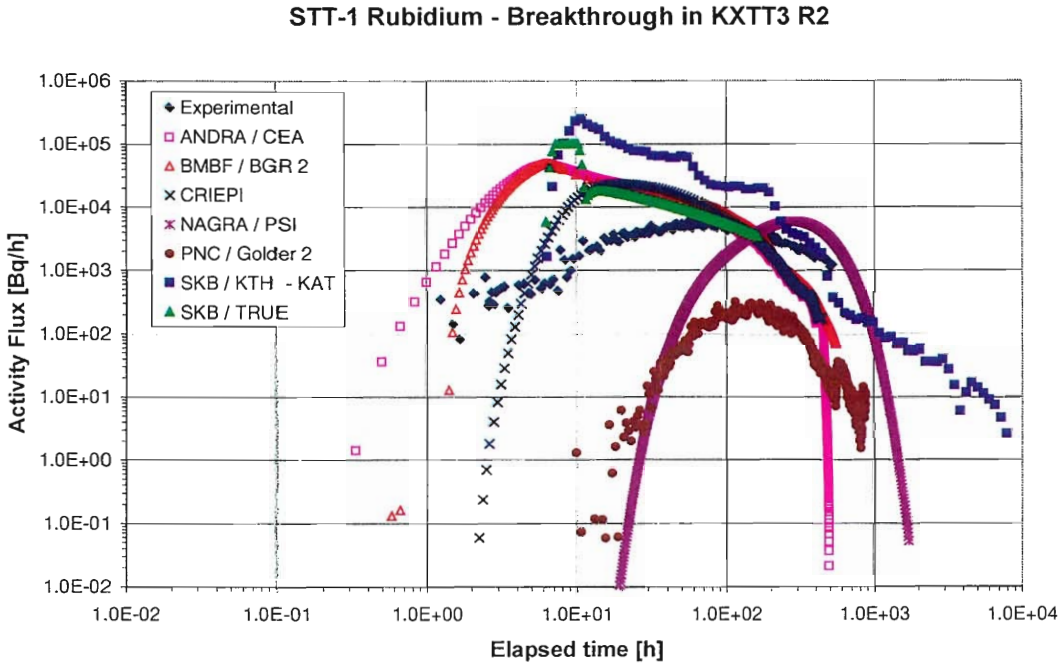
Predictions Sr-85 STT-1

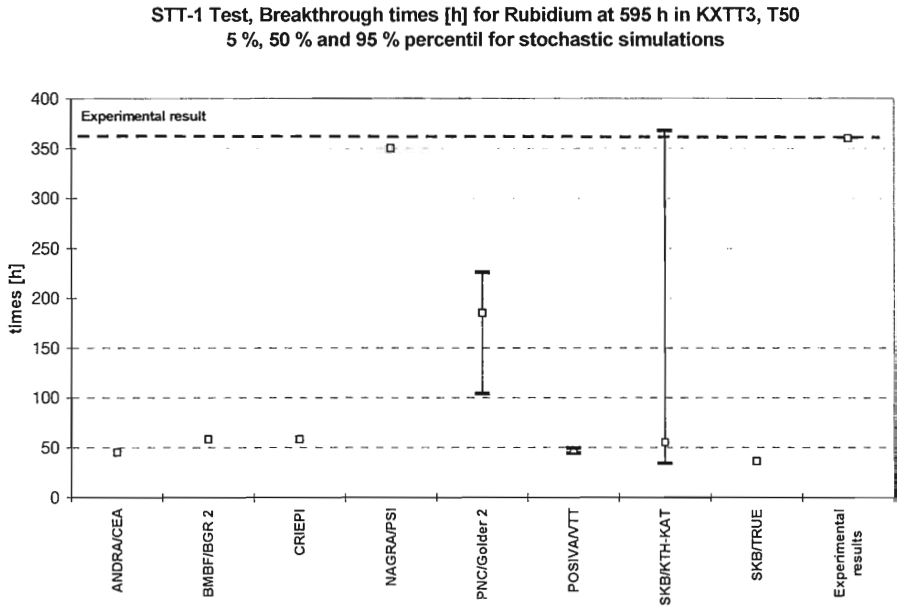




Kemakta

Predictions Rb-86 STT-1

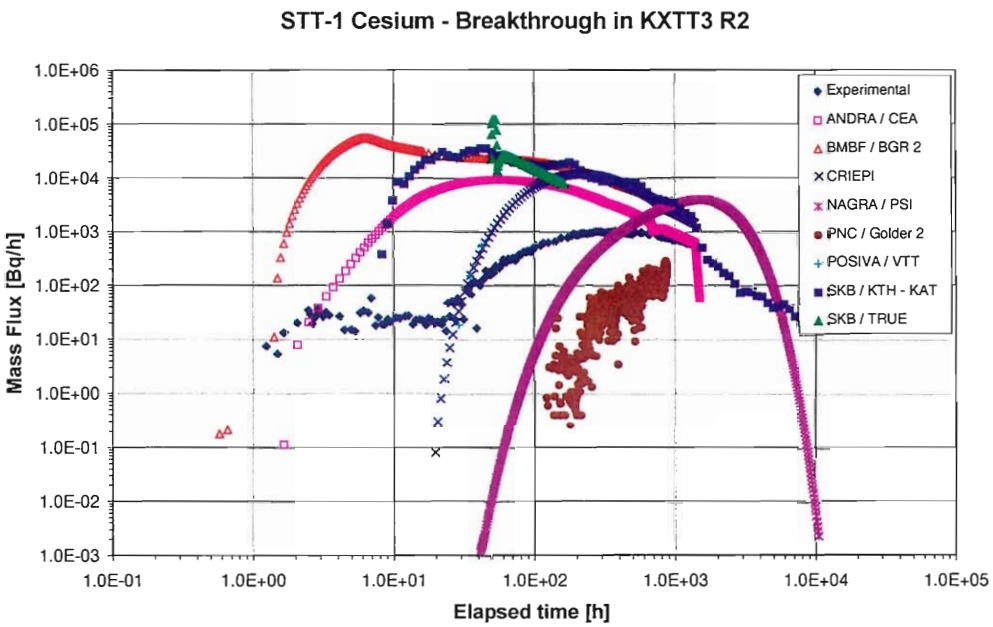


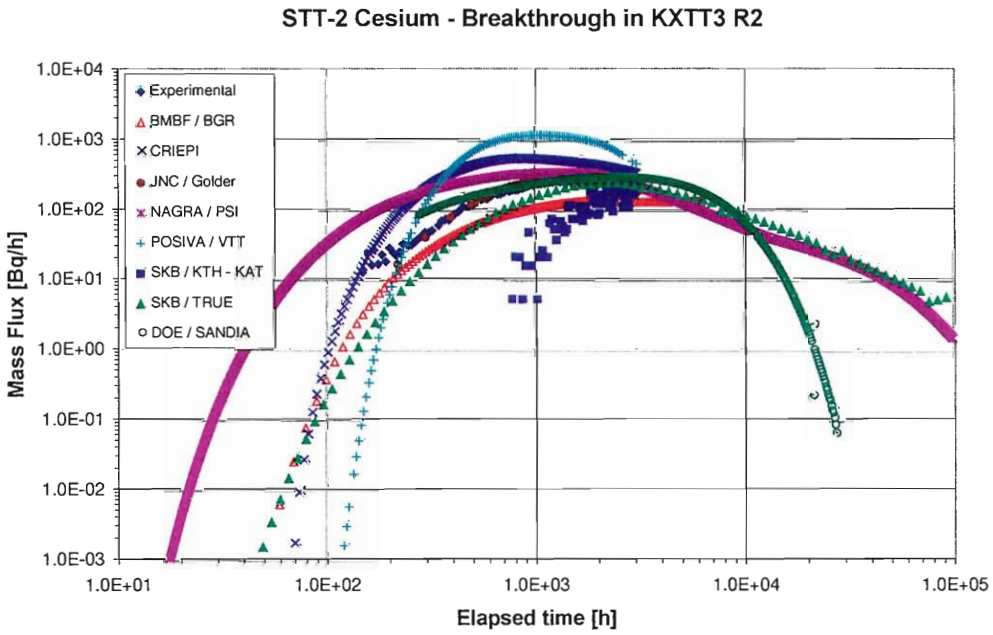


Kemakta

MODIFICATIONS IN MODELS TO ACCOUNT FOR SORBING RADIONUCLIDES									
	ANDRA CEA	**BMWi BGR**	**CRIEPI**	**DOE Sandia**	**JNC Golder**	**NAGRA PSI**	**POSIVA VTT**	**SKB ChE**	**SKB WRE**
STT-1	Surface sorption Matrix diffusion	Surface sorption	Surface sorption		Surface sorption	Surface sorption Diffusion & sorption fault gauge	Surface sorption Matrix diffusion	Matrix diffusion	Surface sorption (matrix diffusion)
STT-1b		+ Matrix diffusion	Increased Ka		+ Matrix diffusion 2 pathways	+ Diffusion in altered rock 2 pathways		Increased Kd*De	+ Diffusion into fault gouge & stagnant water
STT-2	Increased De & specific surface	Increased Ka, Kd	+ Matrix diffusion Adjusted Ka, Kd	Total capacity for mass transfer from STT-1	Adjusted Kd Stagnant zones 9 pathways	Adjusted diffusivities	Adjusted Kd, Ka Channels with varying velocity	Reduced flow rate in flow path	Enhanced diffusion factor

Predictions Cesium STT-1 vs STT-2





Discussion topics

- Calibration and model modifications made for sorbing nuclides between STT-1, STT-1b and STT-2
- Effect of matrix sorption vs. surface sorption
- Effect of gauge material
- Use of laboratory measurements of Kd, Ka, De
- Multiple pathways
- Immobile-mobile zone exchange
- Extrapolation of tracer experiments (non-sorbing tracers - sorbing tracers)
- Specific surface for sorption and matrix diffusion

Deconvolution of Task 4F breakthrough curves

M Elert and H Svensson (Kemakta)

Deconvolution of breakthrough curves STT-2 (Task 4F)

Äspö Task Force meeting

8-11 February 2000

Mark Elert and Håkan Svensson

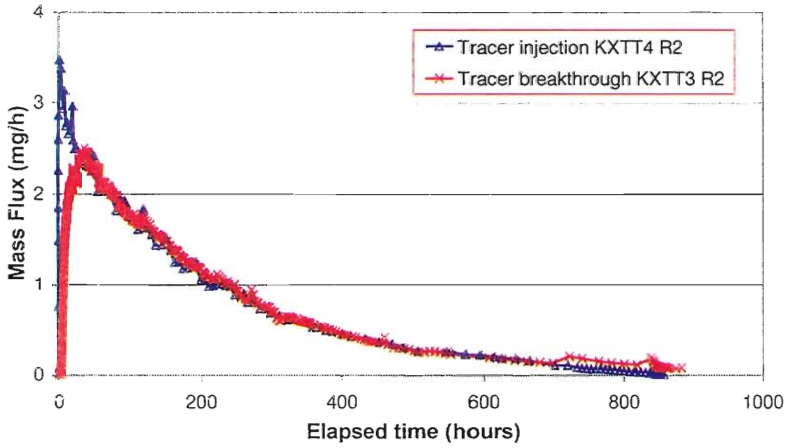
Kemakta Konsult

Introduction

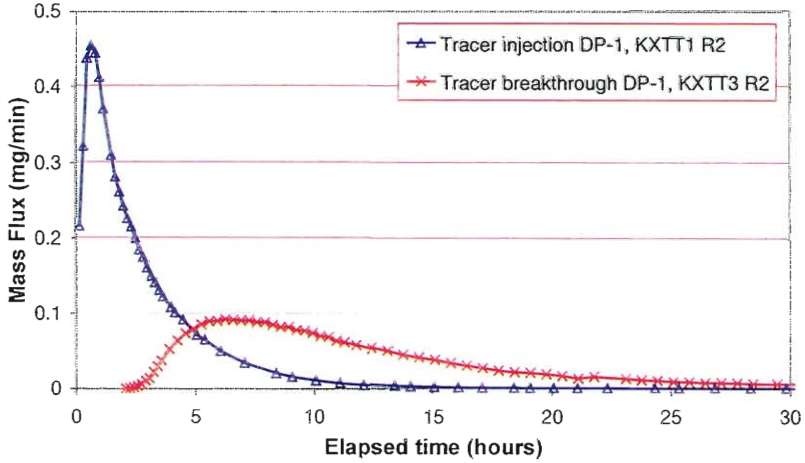
- Short well-defined injection source term beneficial for evaluation of tracer tests
- Proved practically difficult to achieve
- Evolution of injection techniques RC-DP-STT
- Mathematical treatment of experimental data - Deconvolution
  - eliminating the effect of the source term
  - problems with experimental errors
  - oscillations or mathematical artefacts
- Deconvolution of STT-1 and STT-1b
- Deconvolution of STT-2

Injection and breakthrough curves

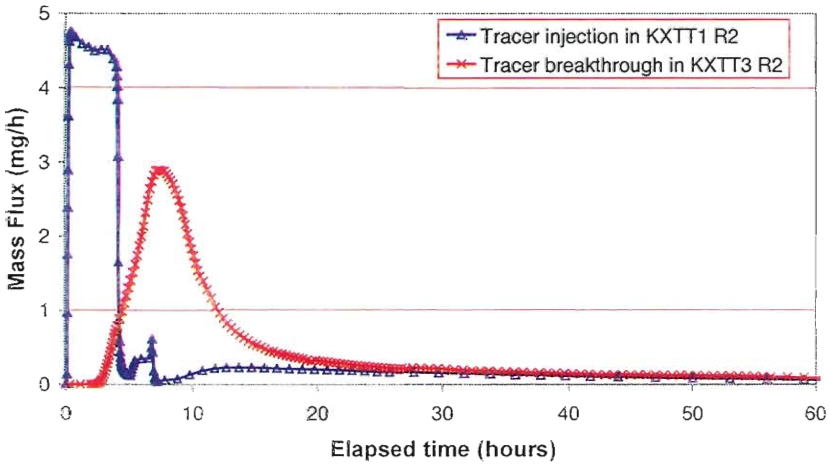
RC-1



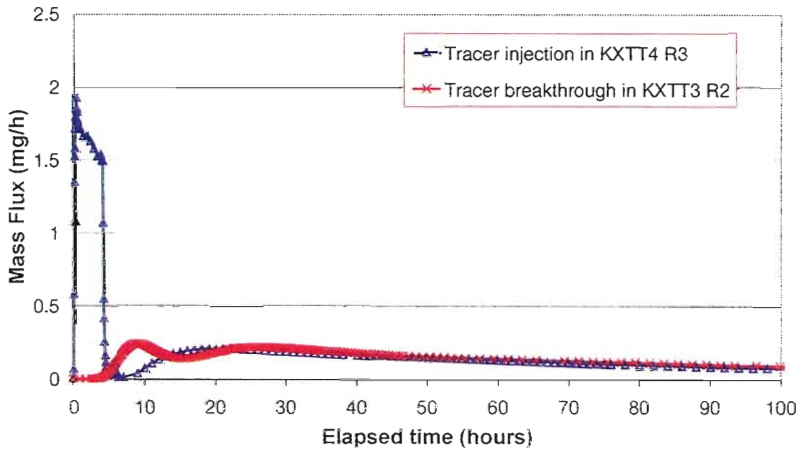
DP-1



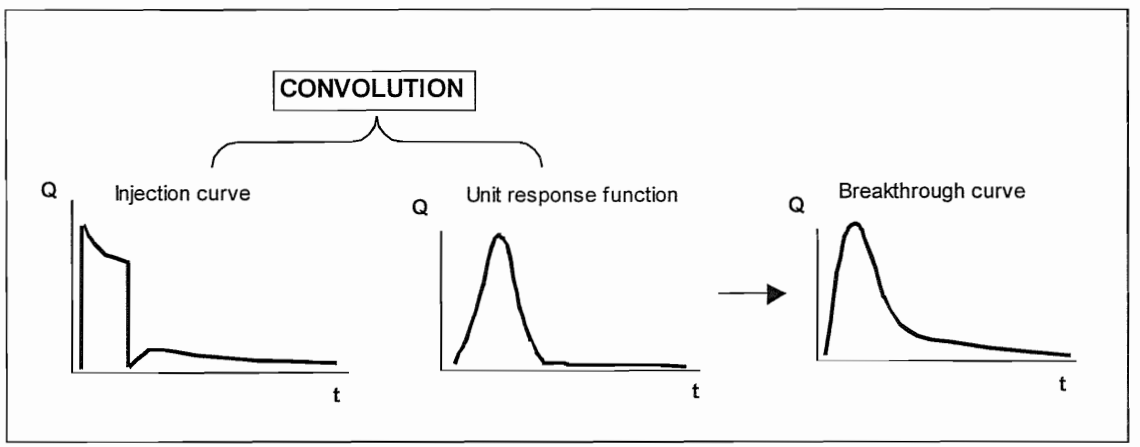
STT-1b



STT-2



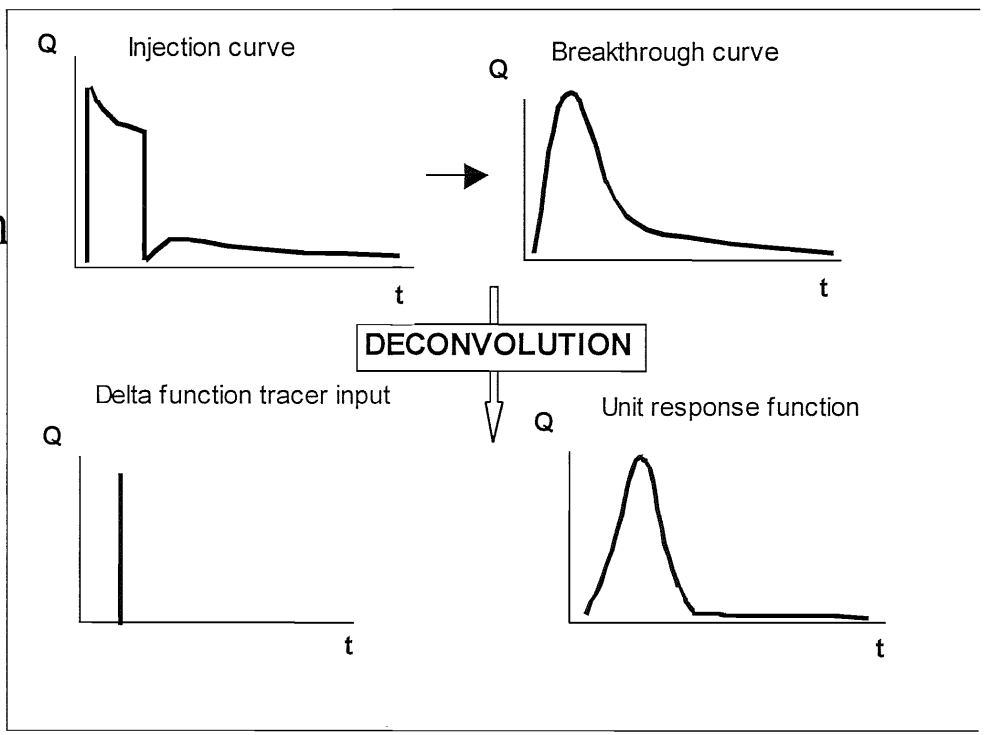
Convolution



- The reverse process of deconvolution
- For obtaining the breakthrough curve for a given injection curve if the unit response function is known

Deconvolution

- Uses the experimental injection curve and breakthrough curve
- Result: a transfer function or unit response function
- Breakthrough curve with input of Dirac delta function (unit mass, zero duration)



Deconvolution techniques

- Deconvolution is an ill-posed problem: small measurement errors may cause severe numerical problems
- **Fourier transform**: Division of Fourier transforms with filtering.
- **Regularisation**: minimising object functions for fit to the solution and properties of the solution (e.g. smoothness)
- **Extreme Value Estimation method** (EVE): solves a linear set of equations where all unknowns are required to be non-negative. Upper and lower band estimates
- **Toeplitz method**: injection and breakthrough as discrete functions. Transfer coefficients defined as a Toeplitz matrix.

Toeplitz method used in this study

- Tracer injection mass flow m_j
- Tracer breakthrough M_i
- Unit response function a_{ij}
- a_{ij} defined as a Toeplitz matrix. Time invariance can be described as a vector.

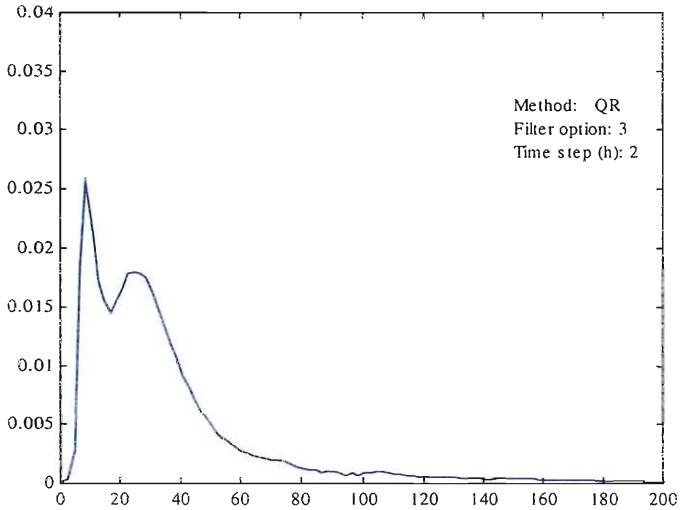
$$M_i = \sum_j a_{ij} \cdot m_j \qquad M_i = \sum_s m_{is} a_s$$

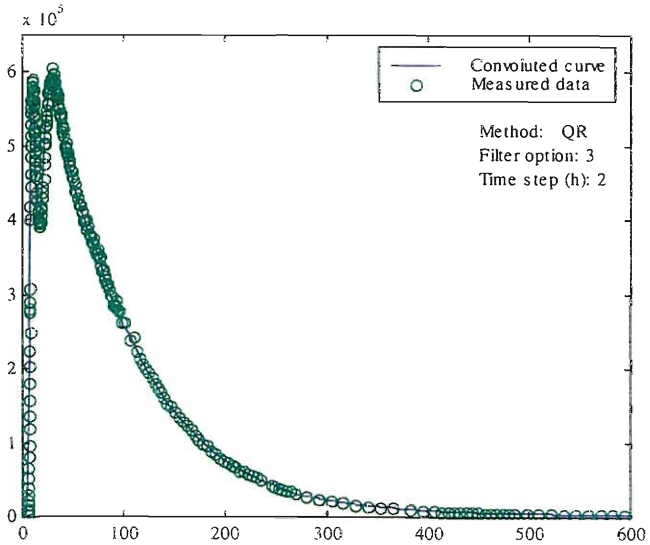
- **M = m•a**
- **a = m^{-1}M**

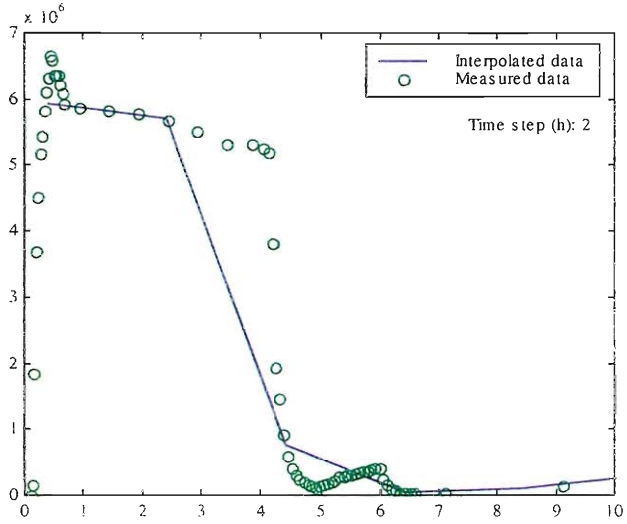
Method used in this study (contd.)

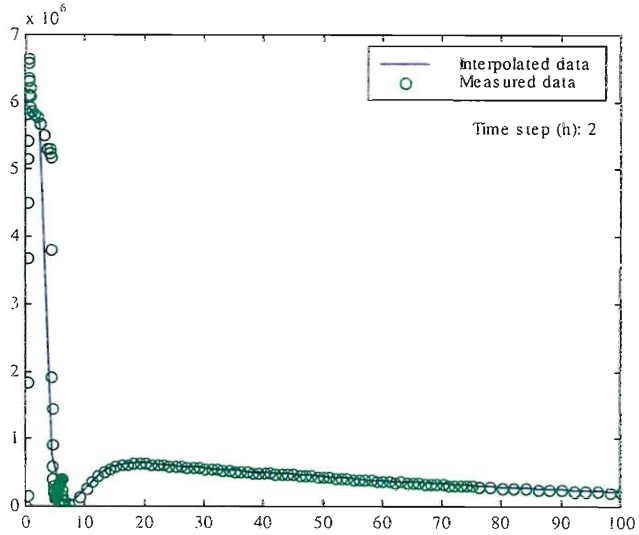
- The Toeplitz method considerably more stable than deconvolution routine of Matlab
- Filtering of breakthrough curves
  - spiky curves were filtered using a moving average filter
  - filter shape and length varied for optimal results
- Convolution of unit response function
  - the result was convoluted with the injection curve and compared with the original breakthrough curve

Deconvolution HTO STT-2

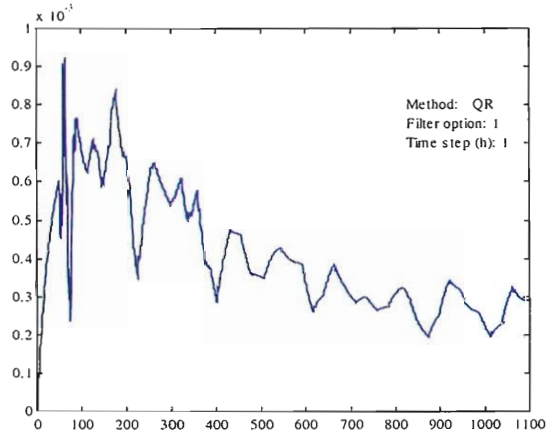


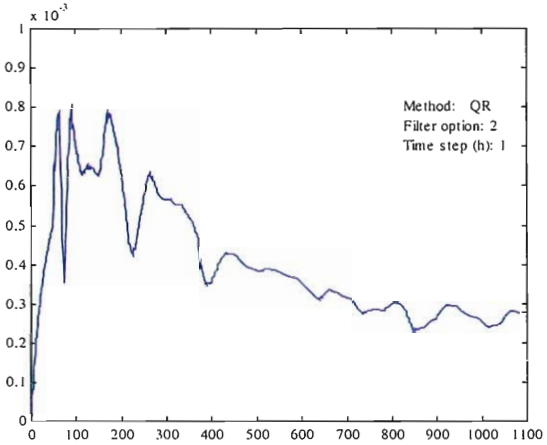


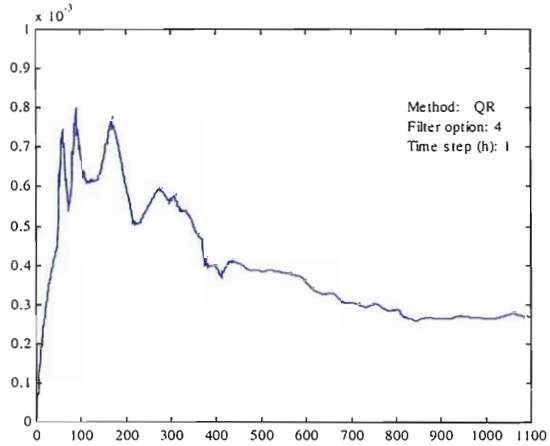


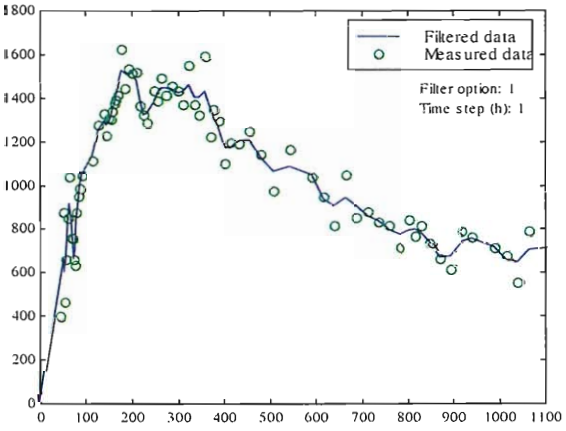


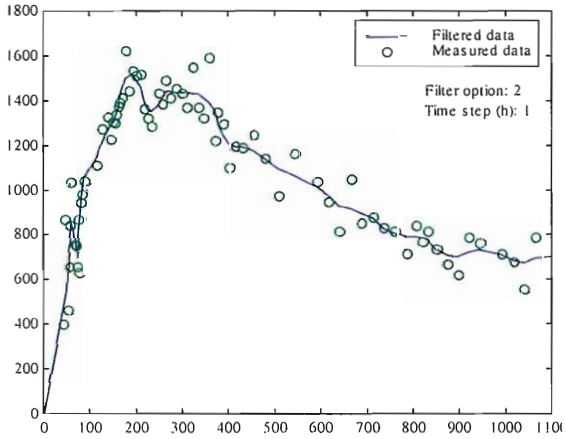
Varying filter length Rb-86 STT-2

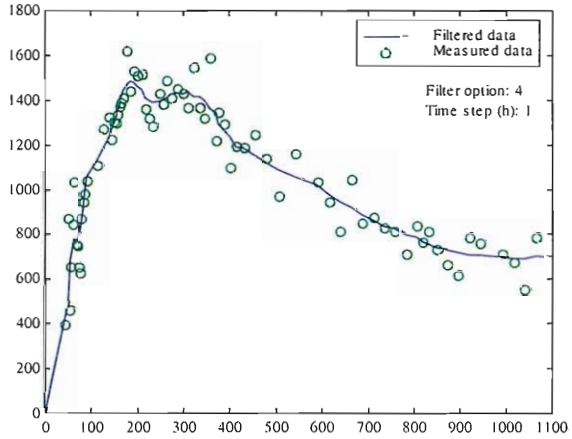




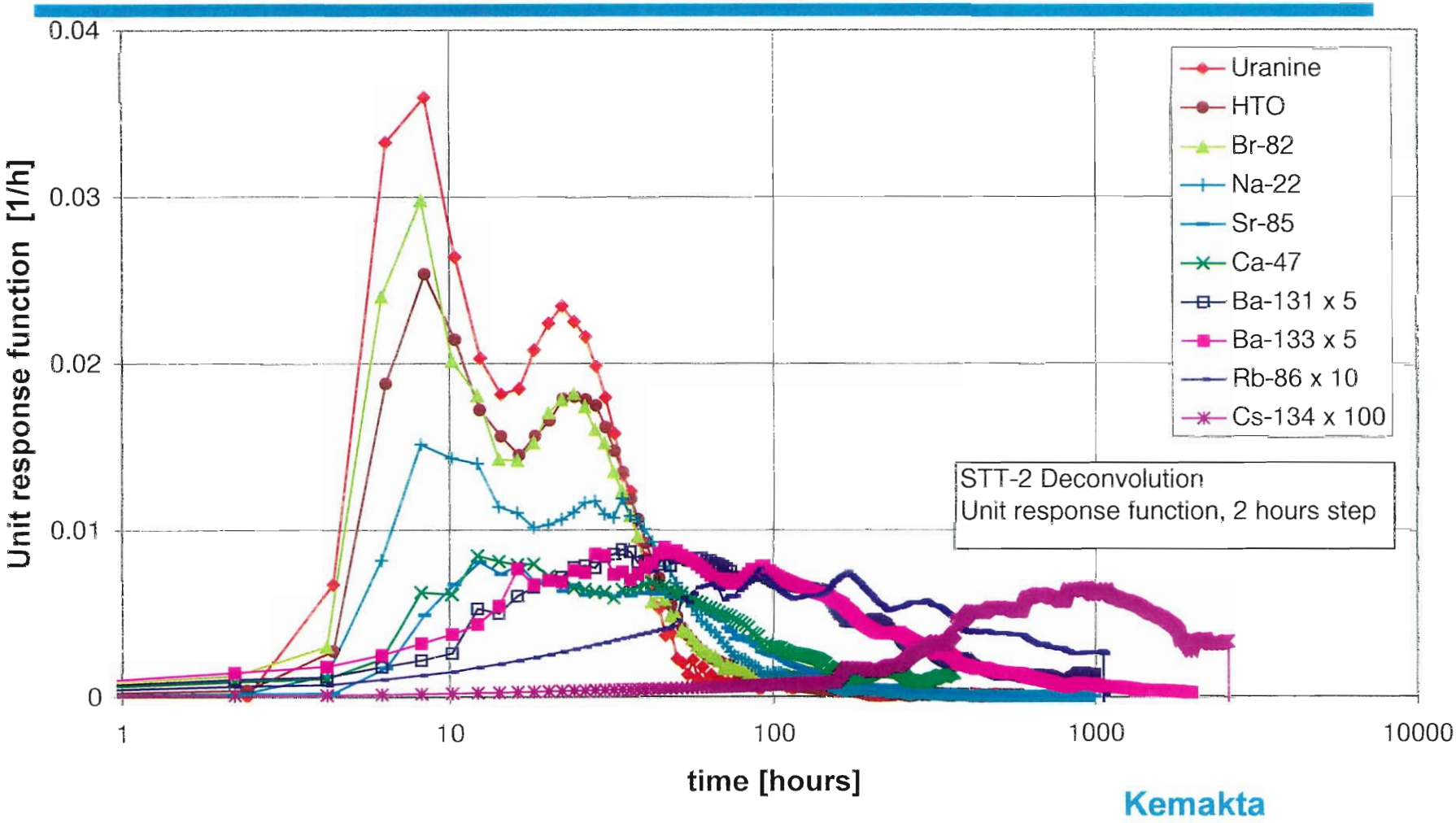








Summary of deconvolution STT-2



Conclusions

- Deconvolution approach helpful when evaluating tracer experiments
  - evaluate features due to transport processes
  - comparisons between experiments with different source term
  - comparison with unit response functions from models
  - numerical problems can cause artifacts
- The method has successfully deconvoluted all tracers used in STT-2
  - more detailed description of non-sorbing tracers
  - no negative values
  - filtering of spiky output data required
  - irregularities in response function for sorbing tracers
- Double peak in response func. $\Rightarrow$ not an effect of injection procedure
- Areas for possible improvement
  - improved filtering methods

On the potential of deconvolution

P Marschall (NAGRA)

On Potential of Deconvolution as Diagnostic Tool for Tracer Test Interpretation

13th International Äspö Task Force Meeting in Carlsbad

February 9, 2000

P. Marschall

Nagra

Outline

- The potential of deconvolution - some general considerations
- Comments on the Task 4E deconvolution approach
- How to proceed? - Some suggestions

The potential of deconvolution

- Some general considerations

Purpose of deconvolution:

- Model identification

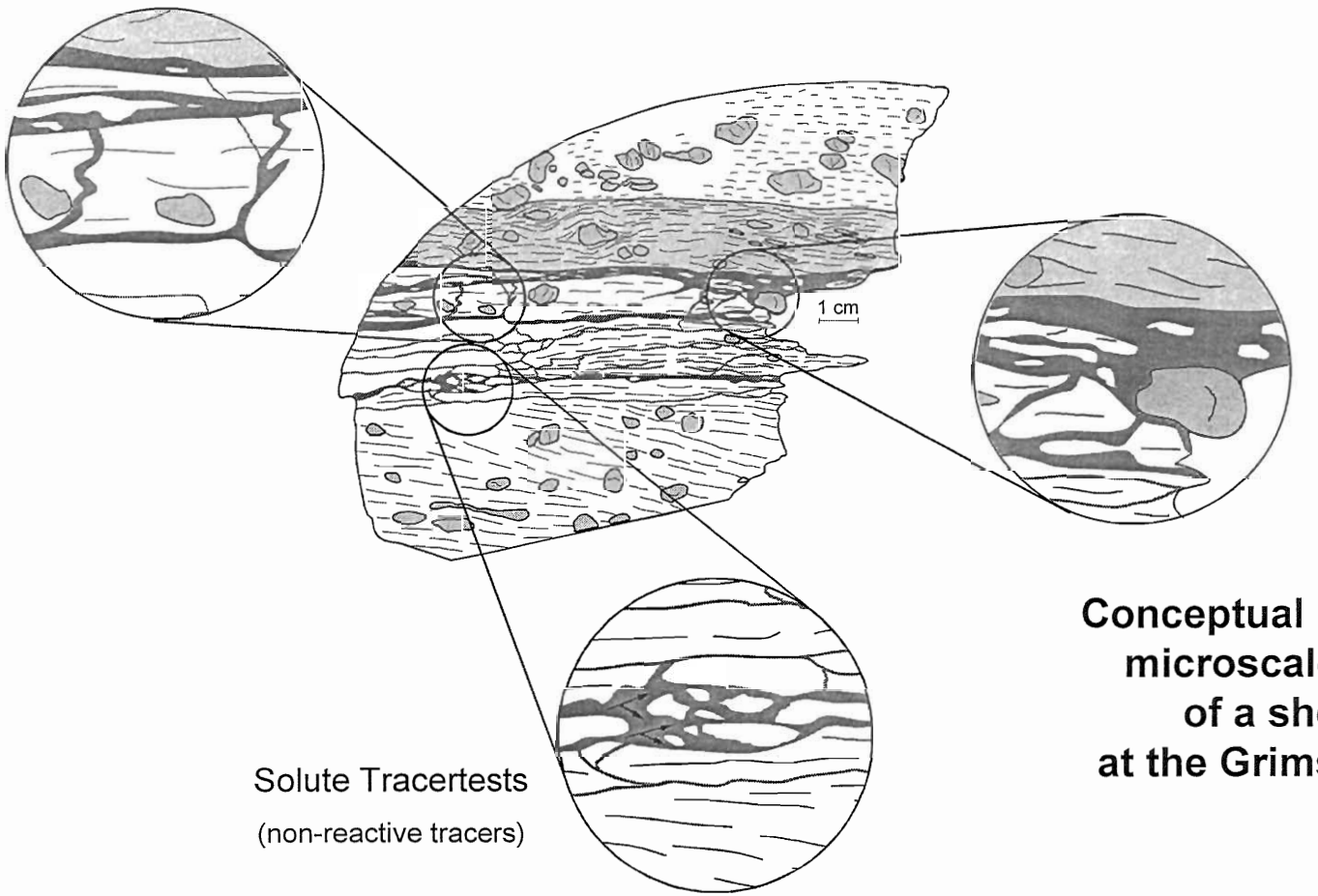
(structure of flow paths, processes)

- Parameter estimation

- Error analysis

The potential of deconvolution

- Some general considerations



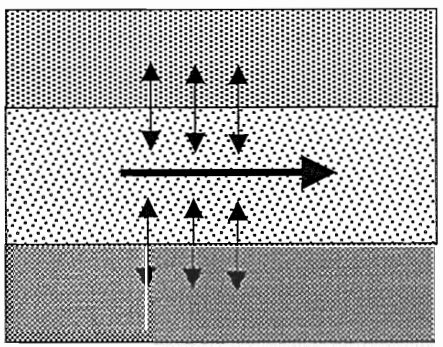
Solute Tracertests

(non-reactive tracers)

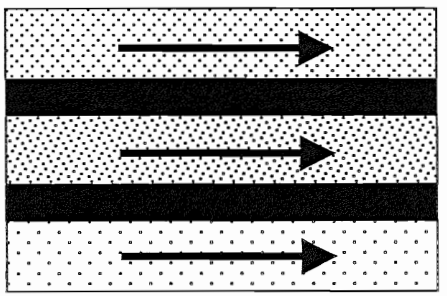
Conceptual model of the microscale structure of a shear zone at the Grimsel Test Site

The potential of deconvolution

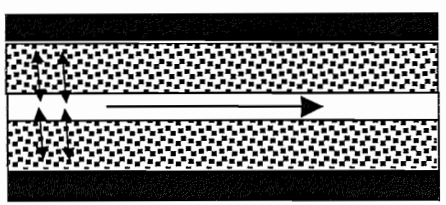
- Conceptual models of solute transport through shear zones



multiple porosity



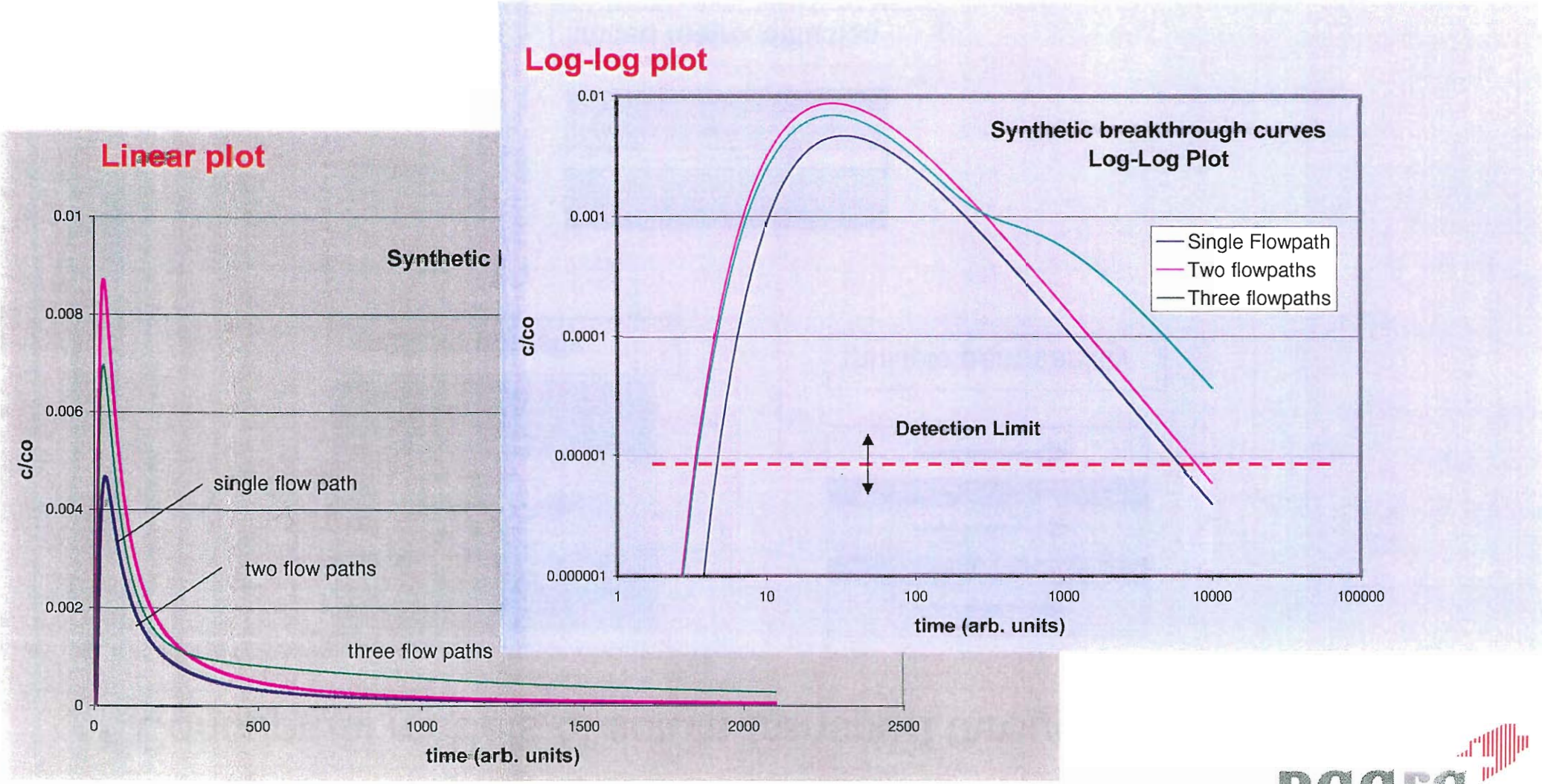
multiple permeability



limited matrix diffusion

The potential of deconvolution

- Diagnostic analyses - the impulse response function IRF



The potential of deconvolution

How to derive the impulse response function?

- Pulse injection

  +immediate diagnostics
  - increased demand on injection techniques
  - restriced resolution in characterisation of higher order porosities

- Injection with heaviside function / deconvolution

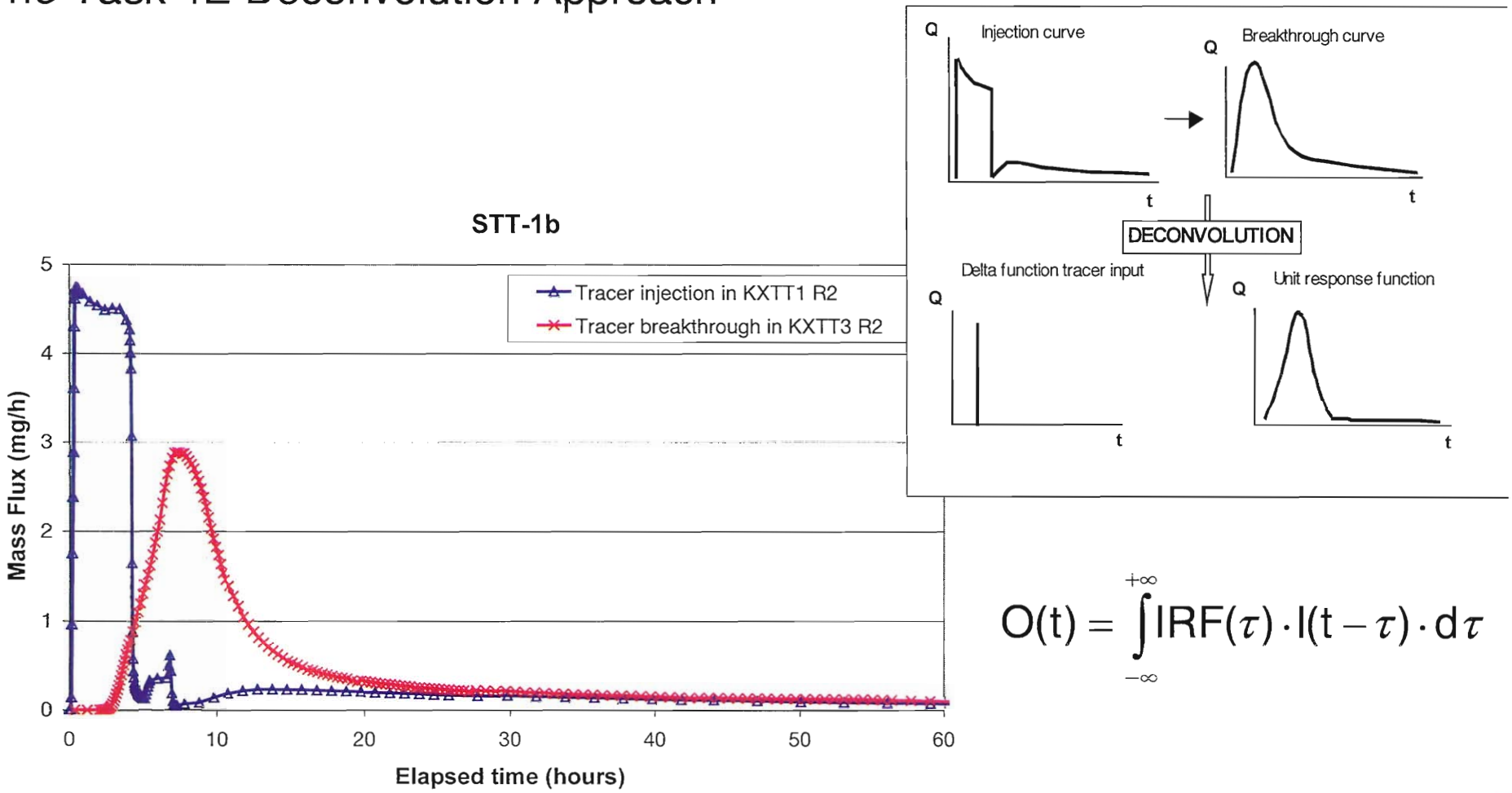
  - an efficient deconvolution approach required
  + less distortion by injection procedure / equipment
  + more focus can be given to higher order porosities

⇒ **Tracer tests with long injection periods are preferred - there is a need for improved deconvolution methods**

nagra

The potential of deconvolution

The Task 4E Deconvolution Approach

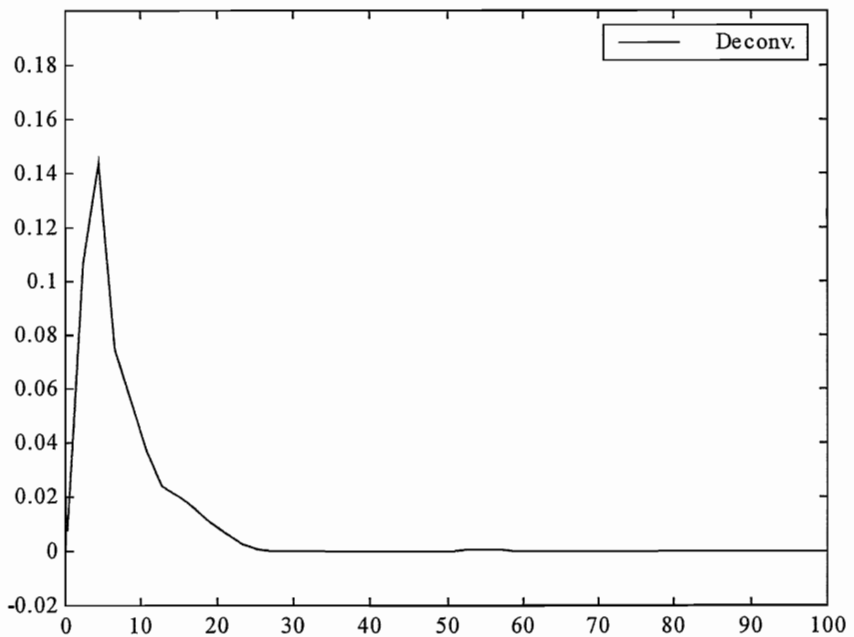


$$O(t) = \int_{-\infty}^{+\infty} IRF(\tau) \cdot I(t-\tau) \cdot d\tau$$

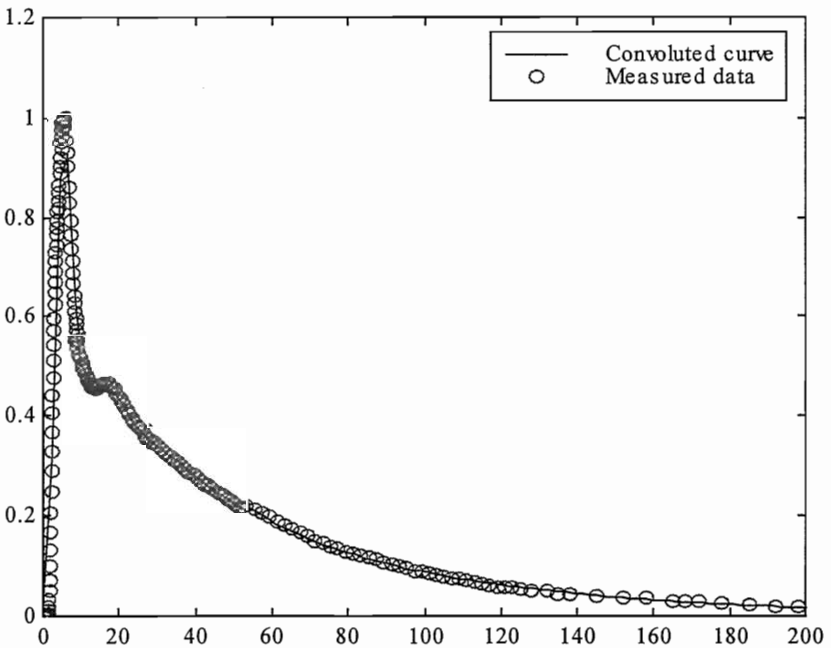
The potential of deconvolution

- The Task 4E deconvolution approach

STT1 - Uranine; IRF from measured data



STT1 - Uranine; IRF * injection conc.

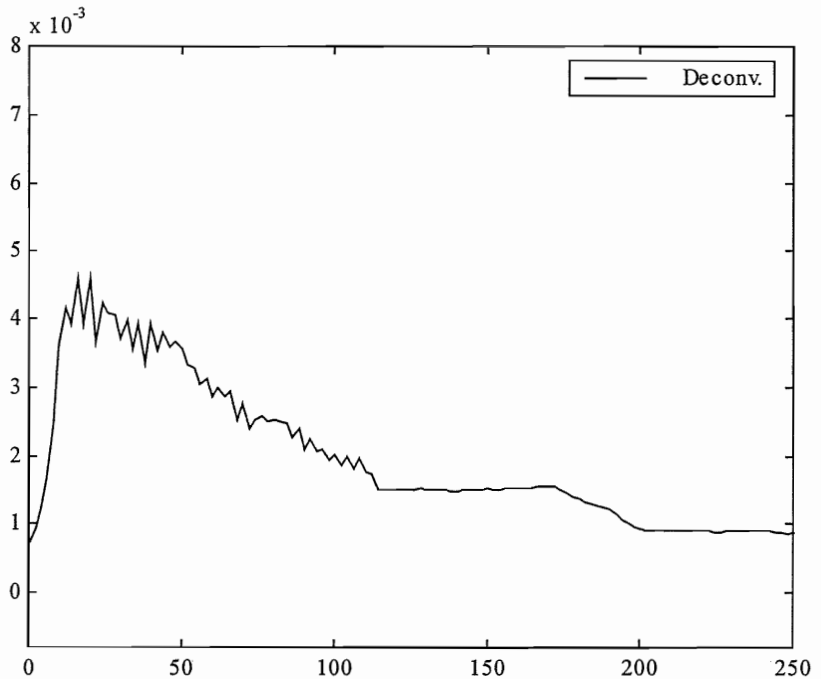


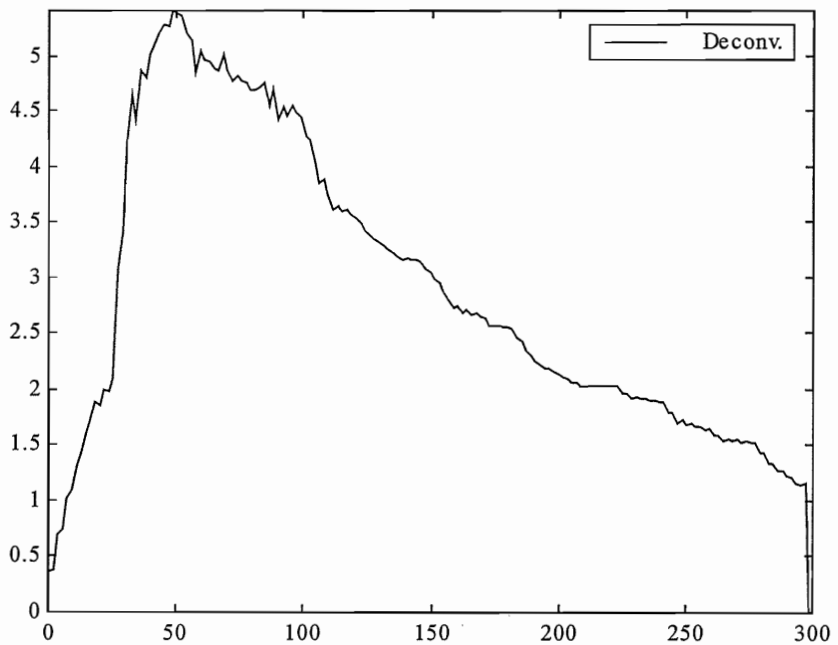
$\Rightarrow$ poor resolution of IRF (i.e. poor process understanding) still leads to acceptable simulation of breakthrough

The potential of deconvolution

- The Task 4E deconvolution approach

STT1 / STT1b - Rb 86; IRF from measured data





$\Rightarrow$ difficulties in treating noise (and non-linearities)

The potential of deconvolution

- How to proceed?

  - Use of suitable base functions / joint analysis of different breakthrough curves

  - deconvolution with non-equidistant (logarithmic) spacing

  - alternative methods (spectral methods, Hankel transforms)

The potential of deconvolution

Suitable base functions

- IRF used in Task 4E

$$M_i = \sum_{j=1}^{m} m_{ij} \cdot IRF_j \qquad \text{where: } t = i \cdot \Delta t, \quad i = 1,m$$

m - input function

M - breakthrough

Number of unknowns: 100 - 1000

- Proposed IRF (assumption: advection/dispersion only)

$$IRF(t) = \sum_{i=1}^{n} \frac{a_i}{\sqrt{b_i t^3}} \exp\left[-\frac{(a_i - c_i \cdot t)^2}{b_i \cdot t} \right]$$

Number of unknowns: 10 - 100

The potential of deconvolution

- Joint analysis of different breakthrough curves

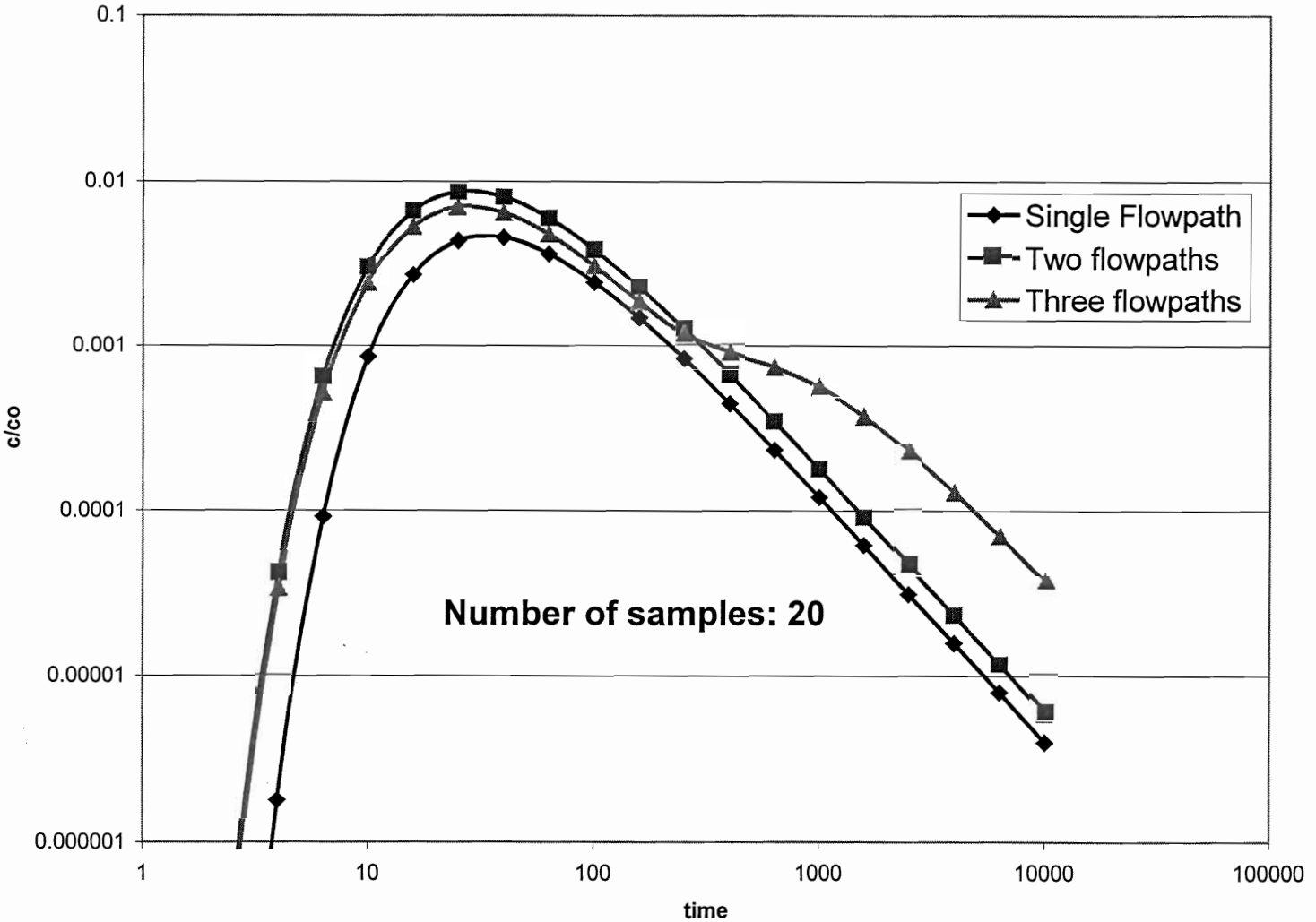
examples:

- conservative tracers with different diffusivities ⇒ dispersion coefficient
- same tracer, different flowfields ⇒ different number of flow paths

⇒ both, using appropriate base functions and joint analysis of a multitude of breakthrough curves leads to more stable inversion algorithms

The potential of deconvolution

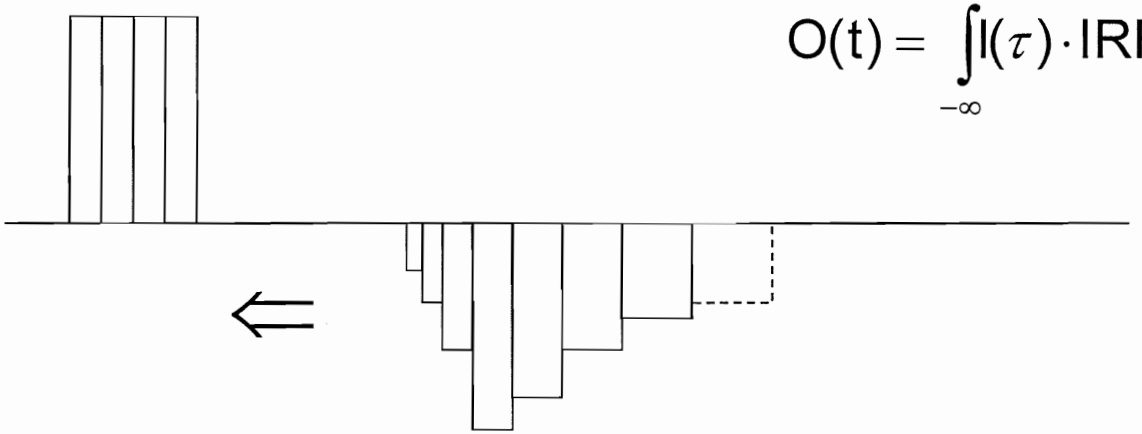
- Non-equidistant spacing / optimised sampling strategies



The potential of deconvolution

- Deconvolution with non-equidistant spacing

Input function I(t)



$$O(t) = \int_{-\infty}^{+\infty} I(\tau) \cdot IRF(t - \tau) \cdot d\tau$$

Logarithmic IRF

Numerical integration techniques required

The potential of deconvolution

- Alternative approaches

  - Hankel transforms

  - Logarithmic Fourier Transforms

  Transfer functions: $T(\nu) = \frac{O(\nu)}{I(\nu)} = \frac{LFT\{O(t)\}}{LFT\{I(t)\}}$

$$IRF(t) = LFT\{T(\nu)\}$$

(Marschall & Schäfer 1994)

To be demonstrated at 14th Task Force Meeting

Resolution of issues and uncertainties in calculations of the transport of radioactive substances

L Liedtke (BGR)

Resolution of issues and uncertainties in calculations of the transport of radioactive substances

Lutz Liedtke - BGR

ABSTRACT

For the long-term safety analysis of a repository for high-level radioactive waste in hard rocks, SKB (Svensk Kärnbränslehantering AB, Sweden) are carrying out a series of in-situ tracer experiments using conservative and reactive tracers in a fairly well defined fracture system, Feature A in the Äspö Hard Rock Laboratory, within the framework of the TRUE-1 (Tracer Retention Understanding Experiment) project, to check and validate the numerical models developed and to determine the transport parameter values in the fractured rock.

Eight modelling groups from seven countries are participating in this project and carrying out the modelling work to support the in-situ experiments. BGR (Federal Institute for Geosciences and Natural Resources, Hanover) utilises the 3D numerical program DURST/Rockflow to simulate the flow and transport processes.

Within the 4C/4D Task, the natural hydrodynamic behaviour and tracer transport processes with conservative tracers in the converging and dipole flow geometry have been evaluated using a deterministic fracture model. Therefore, the fracture geometry, the hydraulic boundary conditions, and the transport parameter values for the conservative tracers have been determined step by step via a set of satisfactory interpretations of the experimental data.

In this report, the reactive chemical processes, radioactive decay and sorption processes (adsorption and desorption) in the fractured rock are discussed analytically, experimentally and numerically within the 4E/4F Task. Based on the results from STT-1 (Sorbing Tracer Test, No. 1), the transport processes of reactive tracers, especially the moderate sorbing tracer, were then modelled using a coupled fracture and matrix model. A satisfactory interpretation of the experimental results for moderate sorbing tracers ^{86}Rb and ^{137}Cs in STT-1/STT-2 was achieved. As a result the matrix effect on sorption and diffusion on the transport processes for the sorbing tracers in the fractured rock cannot be ignored.

ANALYTICAL SOLUTION OF 3-D TRANSPORT EQUATION

The generalised advection-dispersion equation for the transport of chemical substances taking the radioactive decay and the sorption processes into consideration can be written as:

$$n_e \frac{\partial C}{\partial t} + \rho_r \frac{\partial S}{\partial t} + v_a \frac{\partial C}{\partial x_i} = n_e \frac{\partial}{\partial x_i}(D_{ij} \frac{\partial C}{\partial x_j}) - \lambda_c n_e C - \lambda_s \rho_r S, \quad i,j=1, 2, 3,$$

where x_i is the coordinate [m], i=1, 2, 3,
t is the time [s],
$C=C(x_i,t)$ is the concentration of substance in the dissolved phase [kg/m³],
S is the concentration of substance in the sorbed phase [kg/kg],
v_a is the DARCY velocity [m/s],
n_e is effective porosity [-],
ρ_r is the density of the rock [kg/m³],
λ_c is the decay rate of the substance in the dissolved phase [1/s],
λ_s is the decay rate of the substance in the sorbed phase [1/s] and
D_{ij} is the hydro-dynamic dispersion tensor [m²/s].

The tensor D_{ij} can be expressed [Bear, 1972] as:

$$D_{ij} = (\alpha_T |v| + \tau D_m)\delta_{ij} + (\alpha_L - \alpha_T)\frac{v_a^2}{|v|}, \quad i,j=1, 2, 3,$$

where α_L / α_T the longitudinal / transversal dispersivity [m], D_m the molecular diffusion tensor [m²/s], $|v| = \sqrt{\sum v_i^2}$ the velocity [m/s], τ the tortuosity and δ_{ij} the Delta-function.

Assuming that the decay rates in the dissolved and sorbed phases are the same, e.g. $\lambda_c = \lambda_s = \lambda$, and the reaction process can be described after linear HENRY - isothermal relation $S=K_dC$, then the equation (3-6) can be simply rearranged into:

$$\frac{\partial C}{\partial t} + \frac{v_a}{R}\frac{\partial C}{\partial x_i} = \frac{\partial}{\partial x_i}(\frac{D_{ij}}{R}\frac{\partial C}{\partial x_j}) - \lambda C, \quad i, j=1, 2, 3,$$

where $R = 1 + \frac{(1-n_e)\rho_r}{n_e} K_d$ is designated the retardation factor and stays a constant in the case of HENRY - isotherm; K_d is called the distribution coefficient.

The equations has be solved numerically and implemented in the program packet *ROCKFLOW - TM2*.

CONCEPTUAL MODEL

Within the TRUE-1 test site, fractures have been identified on the basis of data from the five boreholes KXTT1 - KXTT4 and KA3005A. All fractures have a dominant NW orientation with a steep dip, corresponding to a major fracture zone, so that it is assumed that the fracture system in the test site may have a hydraulic connection to sea level.

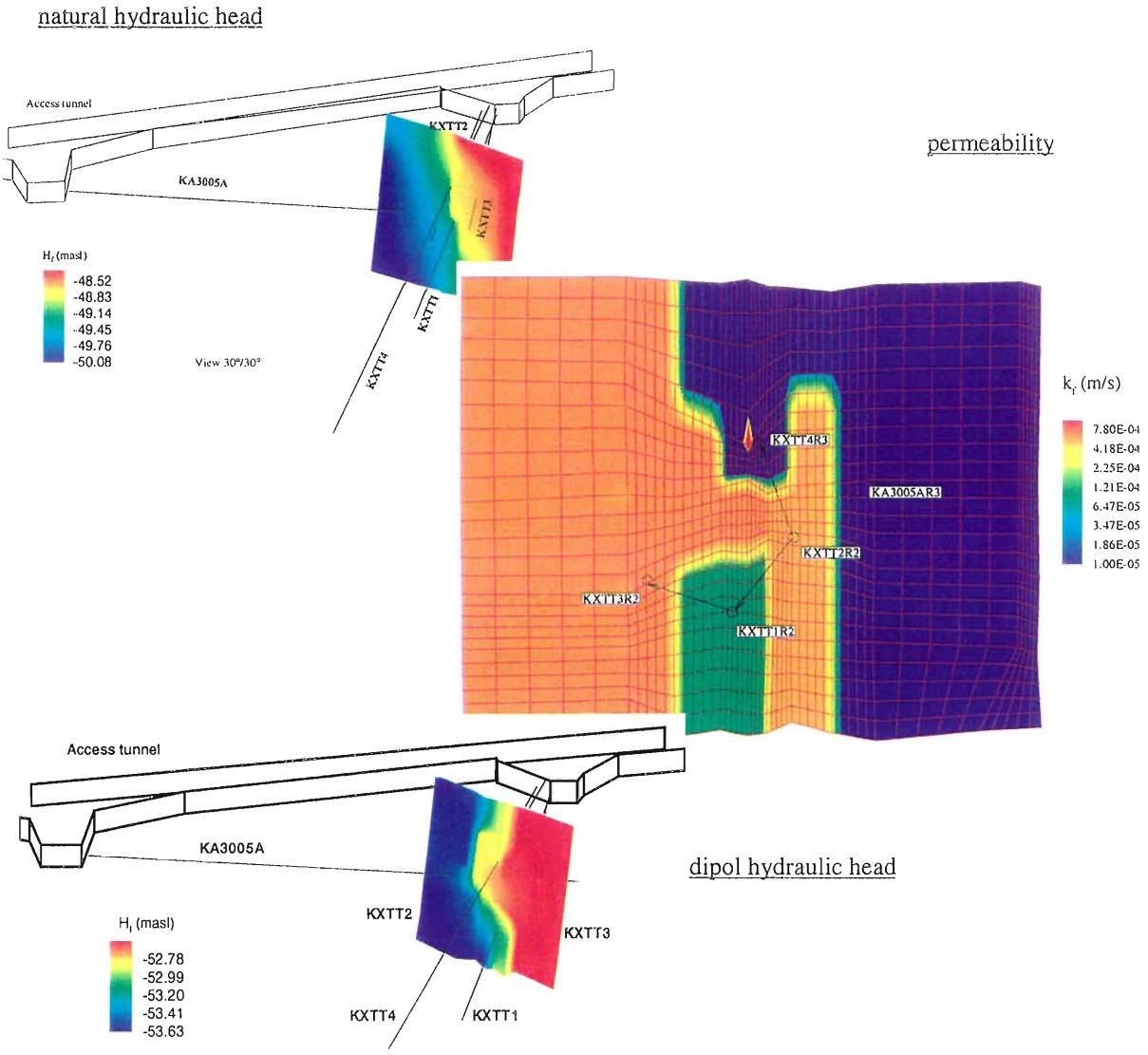


Fig. 1: Natural hydraulic head-, dipol head- and permeability distribution in Feature A (inhomogeneous fracture model)

The potentially water-bearing fractures identified in five boreholes were analyzed based on the deterministic description of the features. Different fracture system features have been classified. Applying the analysis of the geological structural model in the TRUE site Feature A was interpreted as a single, steeply dipping NW trending plane structure. [Liedtke & Shao, 1998] (Fig 1).

FRACTURE MODEL

A single fracture model which was considered as heterogeneous by using a non-constant distribution of fracture aperture and hydraulic conductivity was established to carry out TRUE4C/4D [Liedtke & Shao, 1998] (Fig.2). A satisfactory agreement between the predicted breakthrough curve and associated measurements was achieved when modeling the Radially Converging Test RC-1 and Dipole Tests DP#1-4. A fundamental data set for the transport parameter values (e.g. effective porosity, dispersivity) was then determined.

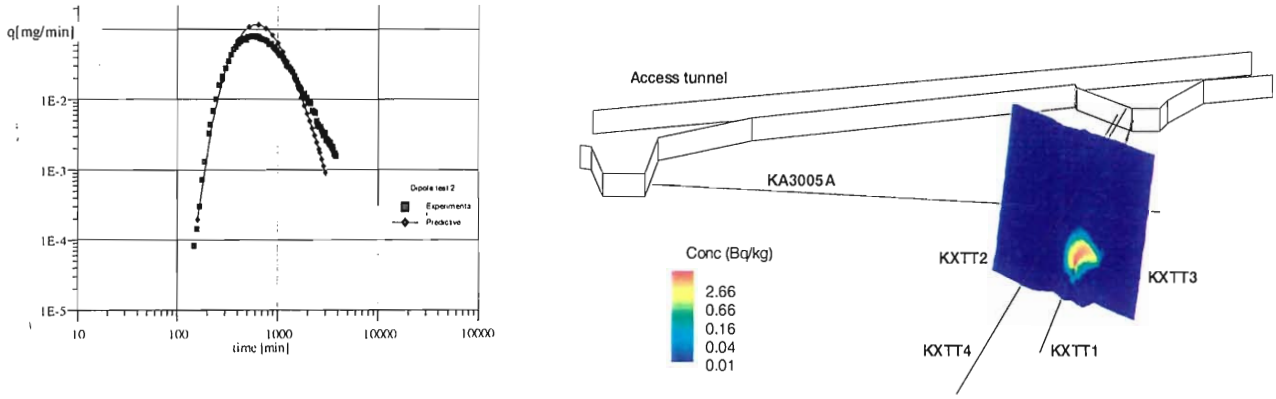


Fig. 2 Distribution of concentration for HTO at the time of 18 h in STT-1b

For the conservative tracer, transport is dominated by advection and dispersion processes, which are determined by flow velocity in the fracture. For a higher flow rate in the injection hole, a relatively fast flow velocity can be realized so that the transport time was restricted to a few days, hence, the influence of the matrix can be ignored (Fig. 2). In this case, a single fracture model can be used to characterize the small scale hydraulic and transport properties in an area like Feature A

.

If the complexity of the tracer test is increased by using sorbing tracer, the single fracture model cannot explain the transport phenomena such as the longer duration of the transport time and longer tailing because the sorption effect plays a major role in the matrix. Variation of the distribution coefficient K_d and numerical diffusion coefficient D in the fracture failed to satisfactorily model the effect of longer tailing in the breakthrough curve (Fig. 3). A coupled fracture and matrix model was therefore developed to model the transport of sorbing tracer.

Coupled fracture and matrix model

In order to find out the size of the sorption effect in the matrix area on the transport breakthrough curve (maximal concentration and breakthrough time) in the case of moderate sorbing tracers, a numerical experiment using a simplified model coupled with 2-D fracture and 1-D matrix was carried out.

Complete 3 dimensional modeling demands considerable CPU time and computer capacity. An analogue model - here called the Brush model - can be employed to estimate transport processes. This model combines 2-D finite elements for the fracture and 1-D finite elements instead of 3-D elements for the matrix (Fig. 5). The advantages of this concept are that the main physical characteristics of the different transport mechanisms in the fracture and the rock matrix are maintained at the same time as dramatically reducing the amount of computer time required. The 1-D elements are localized perpendicular to the fracture plane and coupled to the 2-D fracture elements through common nodes. A chain of 1-D elements is attached to every node of the 2-D mesh. The mass exchange between chains of 1-D elements has thus been deliberately ignored. The cross-sectional area of the 1-D elements is equivalent to the area surrounding the nodes of the corresponding 2-D mesh. Due to the symmetrical geometry, only half of the fracture aperture was considered

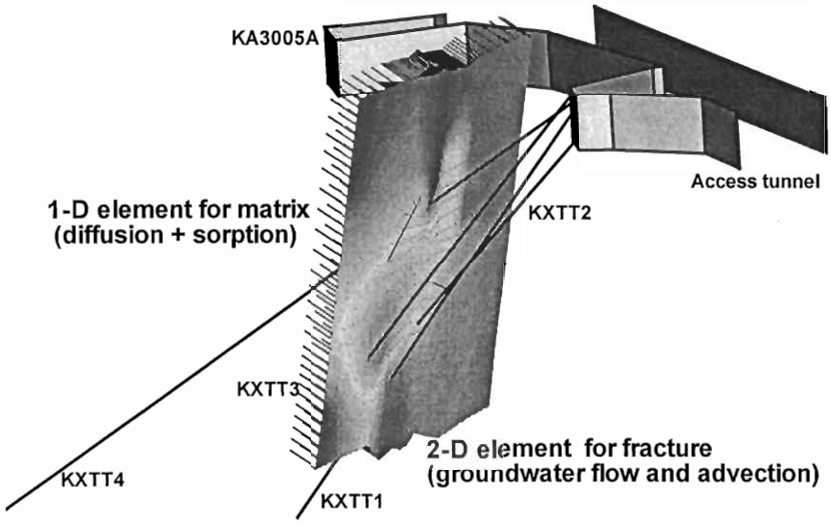


Fig. 3: 1D and 2 ½ D coupled fracture matrix model for Feature A

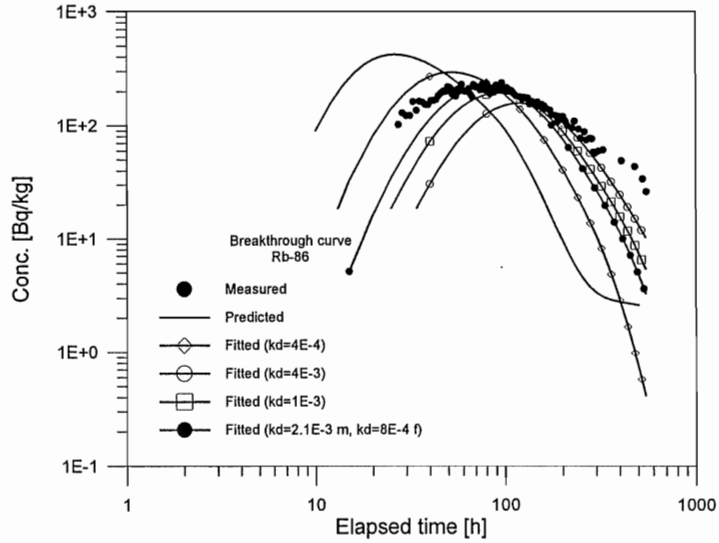


Fig. 4: Influence of the diffusion and distribution coefficients in the matrix on the breakthrough curve in the observation hole

Fig. 4 indicates that the shape of the breakthrough curve for the reactive tracer is different to that of the conservative tracer.

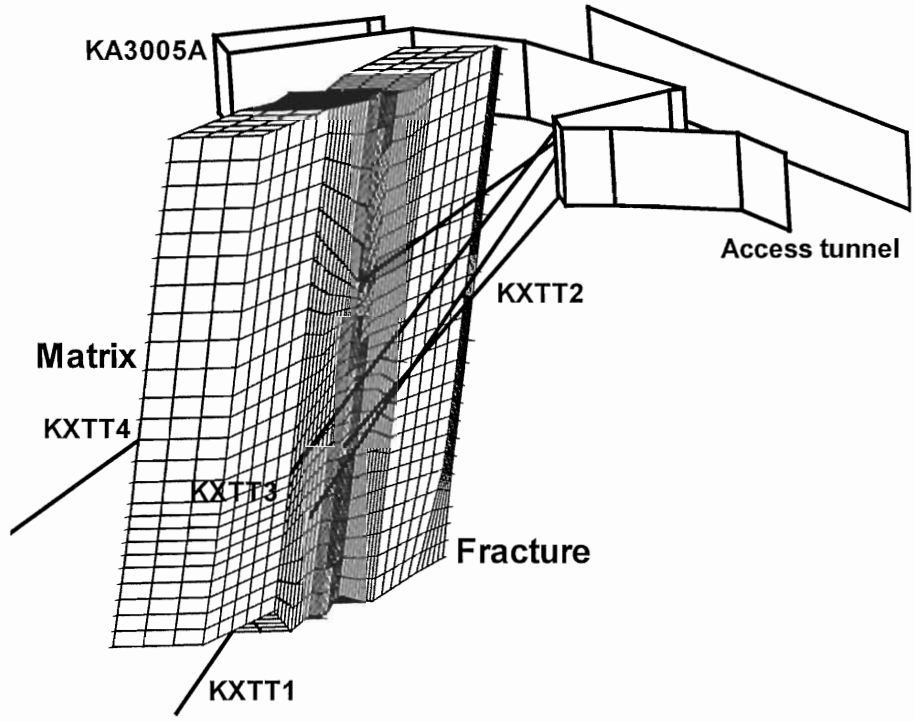


Fig. 5: 3-D coupled fracture matrix model for Feature A in TRUE-4E

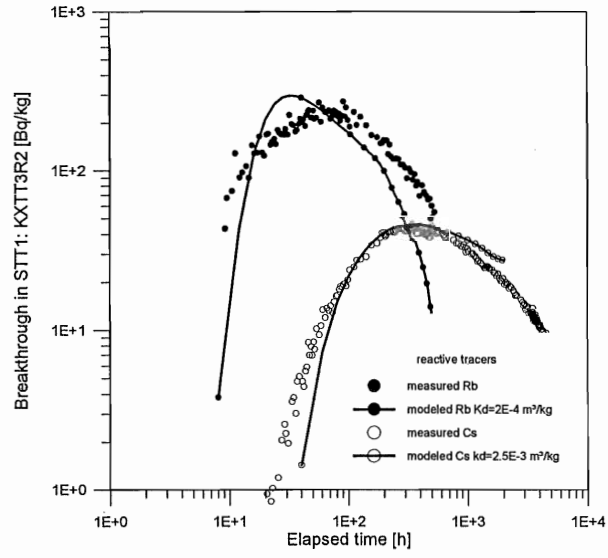


Fig. 6: Comparison of the calculated breakthrough curve using the coupled model with experimental data

The transport time and maximum concentration cannot be obtained by only varying the distribution coefficient in the numerical model. Therefore, a coupled fracture and matrix model was used to interpret the transport processes of the reactive tracers. The fracture properties were not changed in the coupled model with a view to maintaining the consistency of the model and the parameters. The matrix parameter was varied. Taking the natural flow field into consideration, a coupled fracture matrix model, which combined a three dimensional fracture system with a three dimensional rock block, was displayed in Fig. 5. While the parameter values in the fracture remain unchanged, the K_d in the matrix was varied until a best-fit curve was reached (Fig. 6).

As examples, the transport of sorbing tracers (caesium and rubidium) were recalculated using the coupled fracture and matrix model. The parameters used are listed in table 1.

Table 1: Transport parameters used in evaluation of STT-1

Parameter	^{137}Cs	^{86}Rb
Porosity (matrix) [-]	0.01	0.01
Porosity (fracture) [-]	0.3	0.3
Dispersivity [m]	0.9/0.09	0.9/0.09
Matrix sorption K_d [m³/kg]	1.0×10^{-4}	2.0×10^{-4}
Fracture sorption K_d [m³/kg]	2.5×10^{-3}	5.0×10^{-5}
Diffusion [m²/s]	1.0×10^{-7}	1.0×10^{-7}

The recalculation of the tracer tests with weak or moderate sorbing tracers shows that a satisfactory result has been achieved. That means that the rock surrounding Feature A has an influence attributable to adsorption and desorption on the transport time and solute concentration. It makes the transport process slower and reduces the maximum concentration. Table 2 compares the volume / surface distribution coefficient used in the numerical model and quoted from experimental data.

Table 2: Distribution coefficient for casium and rubidium [m³/kg]

	K_a (model)	K_a (laboratory experiment)	K_d (model)	K_d (laboratory experiment)
^{137}Cs	1.0×10^{-3}	5.0×10^{-4} - 1.0×10^{-2}	2.5×10^{-3}	6.0×10^{-3} - 1.4×10^{-2}
^{86}Rb	5.0×10^{-5}	6.0×10^{-5} - 1.0×10^{-3}	4.0×10^{-4}	4.0×10^{-4} - 1.4×10^{-3}

LESSONS LEARNED

- The TRUE-1 site is characterized very well
- In order to determine whether the double peak in the input function is an artifact, the injection technique should be improved.
- The ratio of the recovered mass to the initial mass should be used as a performance measure.
- Measurement of the concentration in the other boreholes and/or in the packer interval in Feature B would provide more detailed information about the tracer distribution in the fracture system.
- Our conceptual model shows that Feature A can be satisfactorily modeled as a planar fracture system. But there may be a channeling effect and this could be described as a one-dimensional element in a two-dimensional model.

RESOLUTION OF ISSUES AND UNCERTAINTIES

- The tracer tests in the Feature A fracture system were interpreted by numerical modeling. The geological model and the numerical model provided a good fit to the measured test data. The tracer transport values (e.g. effective porosity, dispersivity, diffusion coefficient, and distribution coefficient K_d) were determined by modeling various configurations of the tracer tests.
- The numerical models (flow and transport models) have been tested for their suitability for modeling a single-fracture system at the site scale (< 10 m). The question is whether the model and parameters can be scaled up. Extrapolation of the results from site scale to large scale should be investigated in the next step.

CONCLUSIONS

- In such a system it is necessary and very important to determine the fracture geometry and hydraulic patterns under the test conditions. The latter can be determined by iterative modeling of flow and transport.
- Flow and transport parameter values can be determined by numerical modeling of hydraulic and transport tests.
- Sorption and decay properties of radioactive tracers can be modeled numerically.
- Groundwater flow and transport of solutes in the fractured rock can be simulated using the Rockflow program.

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Numerical analysis with FEGM/FERM for Task 4F

Y Tanaka, T Hasegawa and T Igarashi (CRIEPI)

Task4F

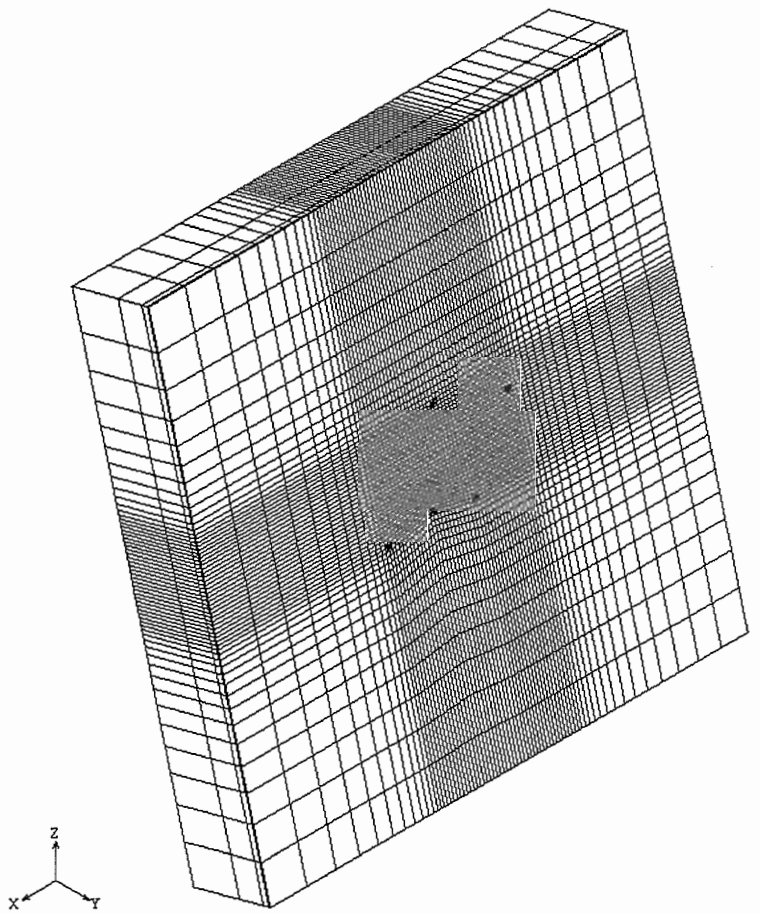
Numerical analysis with FEGM/FERM for Task 4F

Yasuharu Tanaka
Takuma Hasegawa
Toshifumi Igarashi

The 13th Task Force meeting
Feb. 8-10, 2000

CRIEPI

Finite element mesh

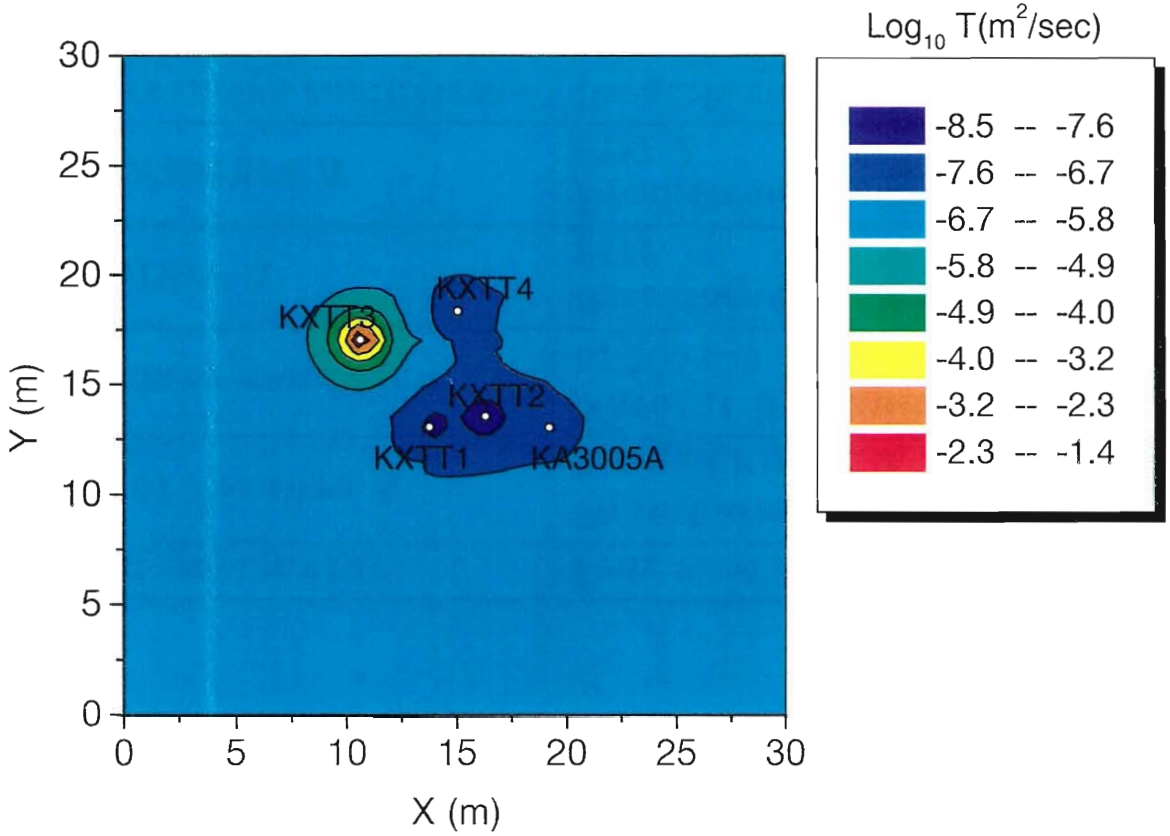


Parameter identification

Identified parameter	Data used for parameter identification
Transmissivity of Feature A	Drawdowns during RC-1, 2, DP-1, 2, 3, 4, 5, 6 and PDT-1, 2, 3
Hydraulic boundary condition	Natural hydraulic head prior to start of PDT-3
Aperture of Feature A	Breakthrough curve of Amino-G during PDT-2
Dispersivity in Feature A	Breakthrough curve of Amino-G during PDT-2
Surface related sorption coefficients	Breakthrough curves during STT-1a
Dispersivity in rock matrix	Breakthrough curves during STT-1a
Matrix sorption coefficients	Breakthrough curves during STT-1a
Fluid flux through KXTT4 R3	Injention curve of Uranine during STT-2

Task4F

Spatial distribution of transmissivity in Feature A estimated by kriging



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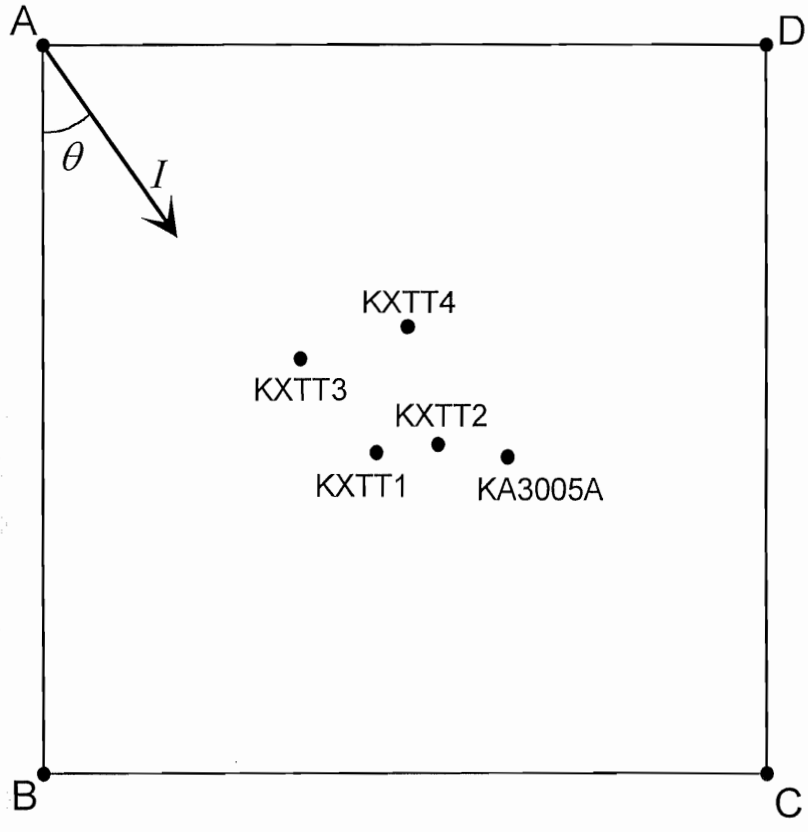
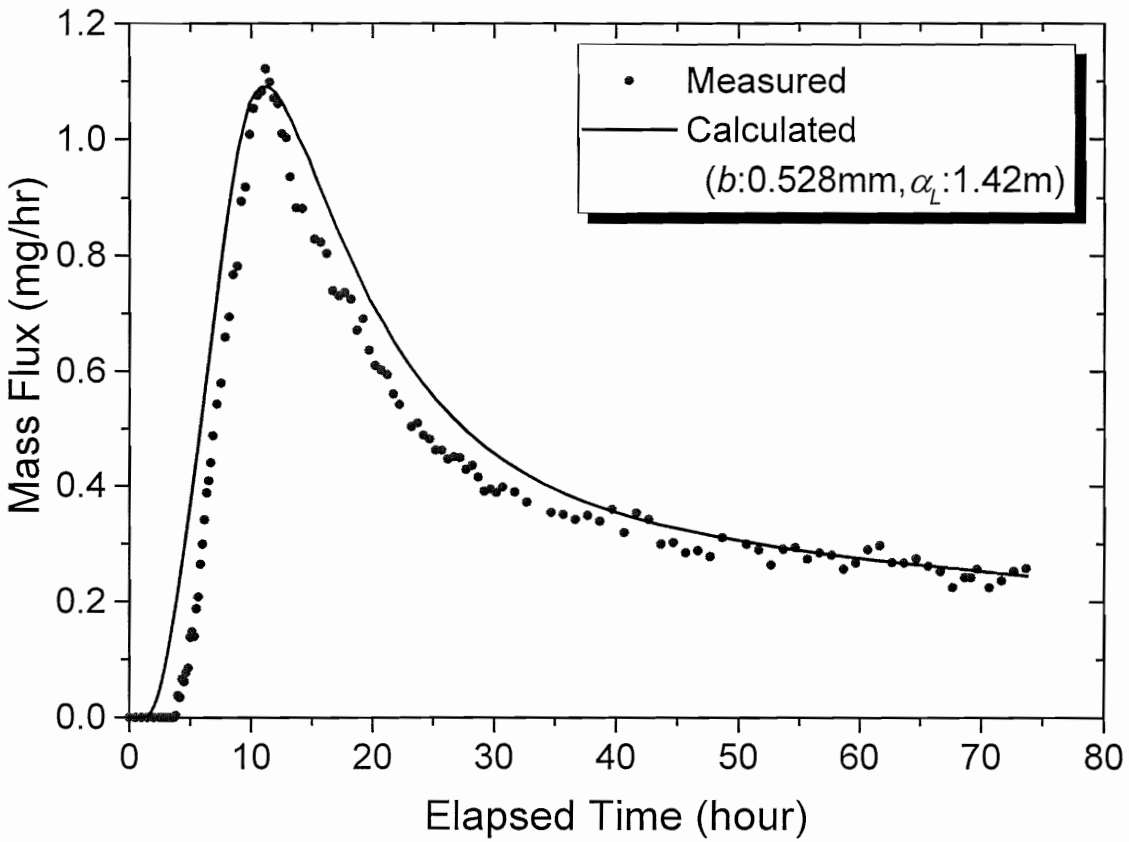
Natural hydraulic head prior to start of PDT-3

Parameters	Identified value
Hydraulic head, h_A	-51.7mH_2O
Magnitude of hydraulic gradient, I	0.124
Direction of hydraulic gradient, θ	57.8°

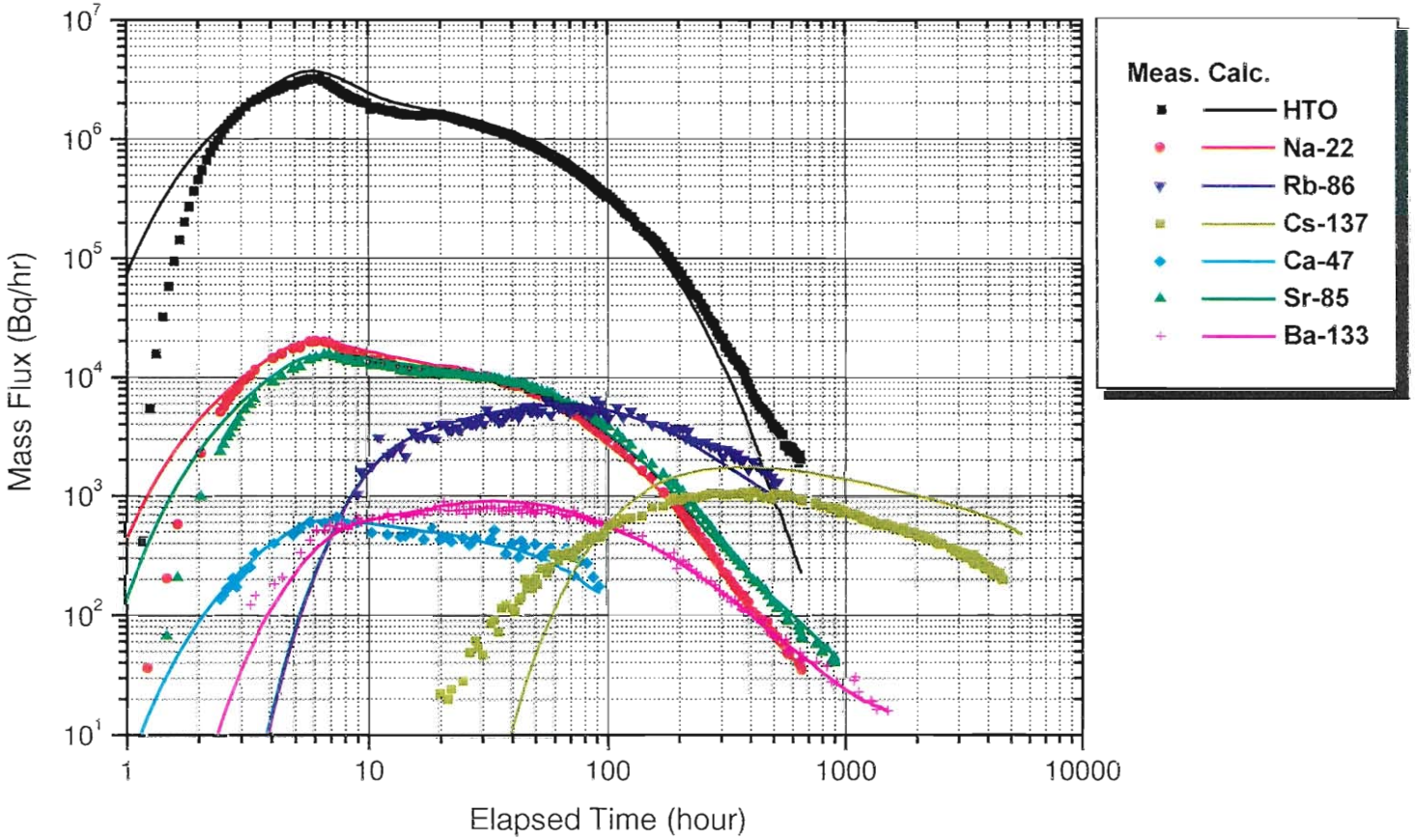


Breakthrough curve in pumping section during PDT-2



Task4F

Best-fit runs of breakthrough curves during STT-1a



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Transport parameters for best-fit runs of STT-1a

Tracer	K_a (m)	K_d (m^3/kg)	D_e (m^2/s)
HTO	-	-	4×10^{-14}
Na-22	4.0×10^{-5}	2.60×10^{-5}	2.2×10^{-14}
Rb-86	1.5×10^{-3}	2.80×10^{-3}	3×10^{-14}
Cs-137	4.5×10^{-3}	6.00×10^{-2}	3×10^{-14}
Ca-47	1.5×10^{-4}	4.16×10^{-5}	1.3×10^{-14}
Sr-85	1.2×10^{-4}	8.00×10^{-5}	1.3×10^{-14}
Ba-133	6.53×10^{-4}	8.00×10^{-4}	1.4×10^{-14}

Injected mass flux of tracer

Fluid flux through tracer injection section, Q_{bh}

$$Q_{bh} = -\frac{V}{t} ln(C / C_0) - Q_{sam}$$

(Winberg, 1996 and Andersson, 1996)

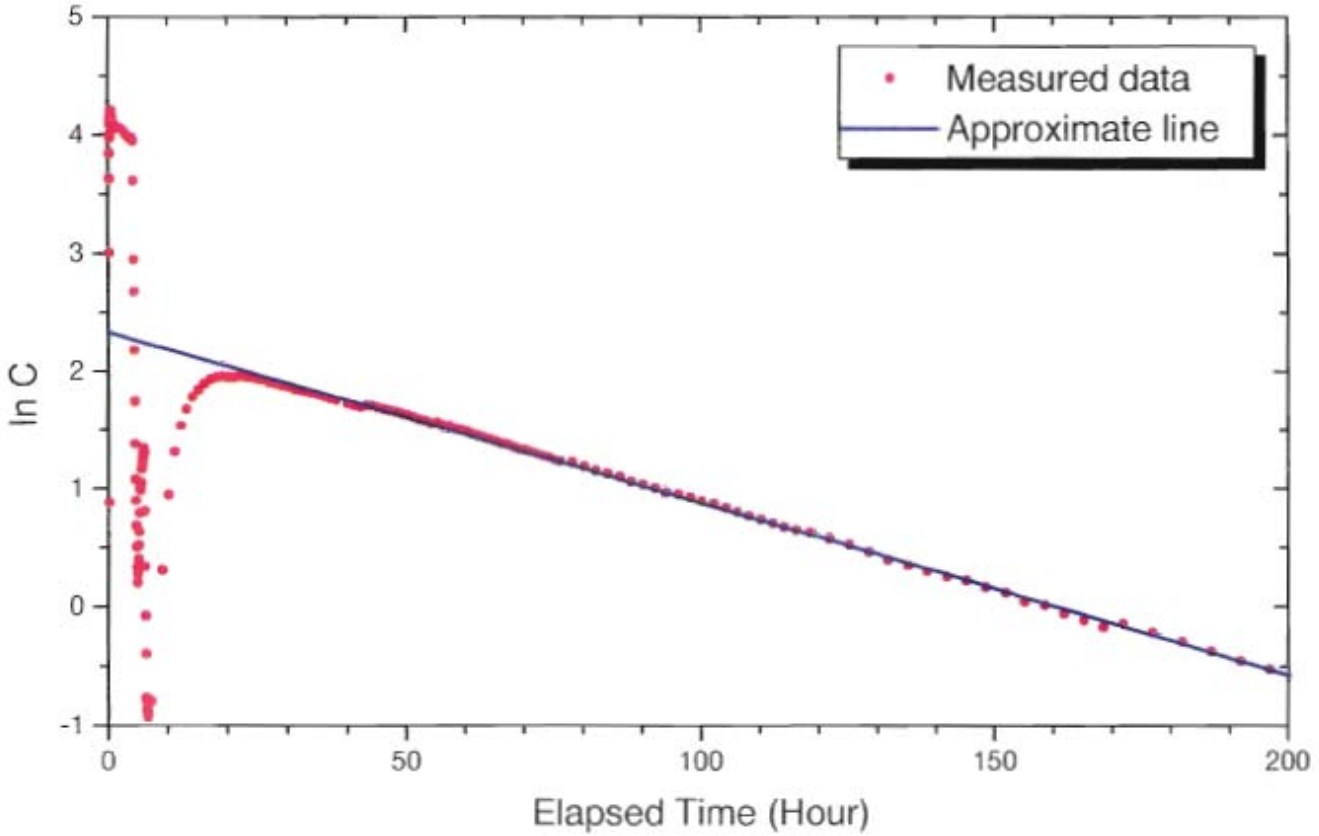
Injection mass flux used for simulation, F

$$F = C \times Q_{bh}$$

Test#	Inj. section	Tracer	Elapsed time (h)	Fluid flux (ml/min)
STT-1a	KXTT4 R3	Uranine	20-70	0.720
			70-200	0.550
		HTO	20-70	0.698
			70-200	0.544
PDT-2	KXTT4 R3	Amino G Acid	10-72.3	0.151
STT-2	KXTT4 R3	Uranine	25-200	0.478
		HTO	25-200	0.486

Task4F

Concentration of uranine in injection section during STT-2



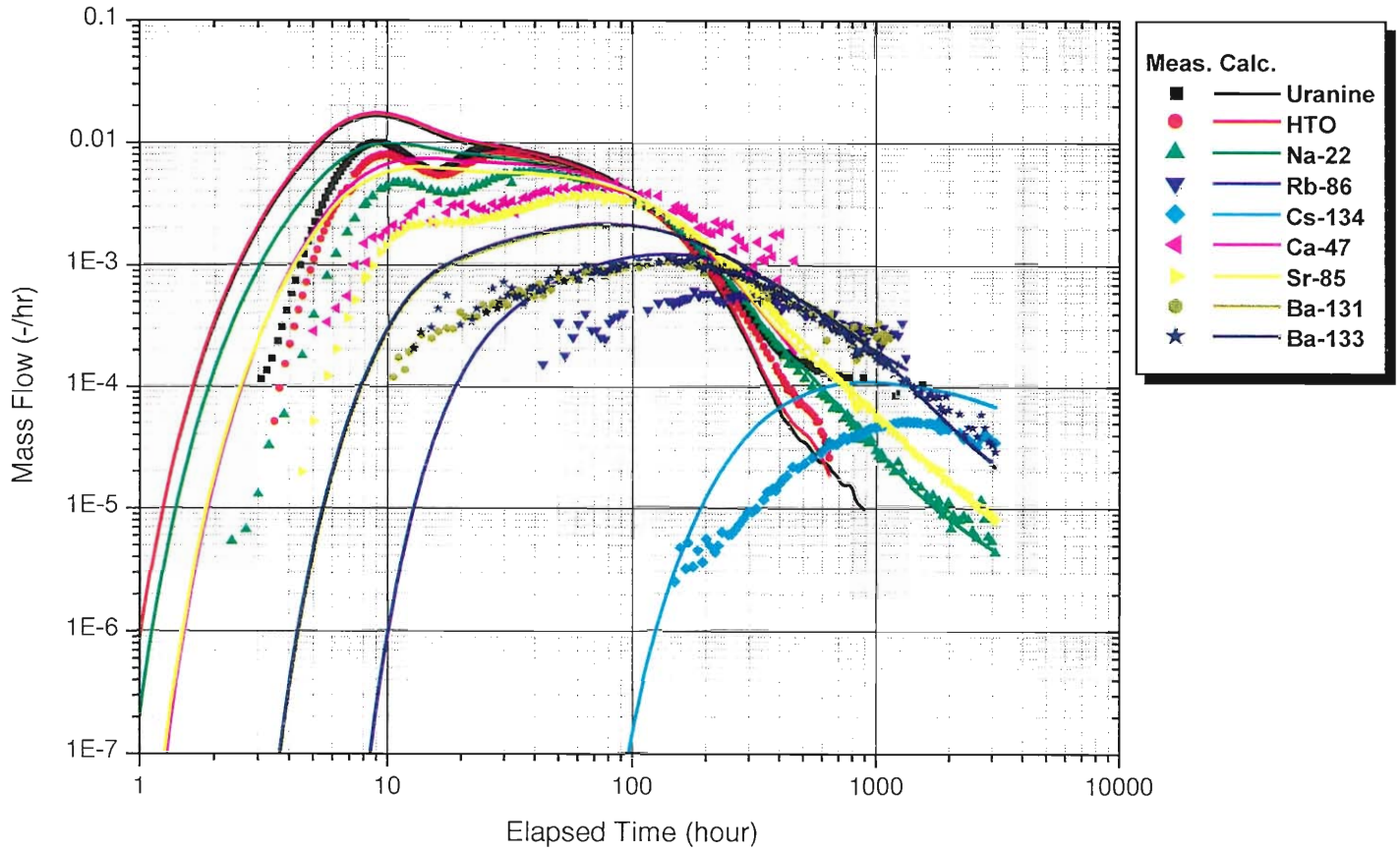
CRIEPI

Parameter values used for simulations of STT-2

Transmissivity of Feature A	KXTT1 R2	9.40e-9 m²/s
	KXTT2 R2	3.81e-9 m²/s
	KXTT3 R2	6.59e-2 m²/s
	KXTT4 R3	2.26e-8 m²/s
	KA3005A R3	4.20e-8 m²/s
Aperture of Feature A		5.28e-4 m
Dispersivity in Feature A	Longitudinal	1.42 m
	Transverse	0.142 m
Permeability of rock matrix		1e-10 m/s
Porosity of rock matrix		0.001
Dispersivity in rock matrix	Longitudinal	0.5 m
	Transverse	0.25 m

Task4F

Mass flow for measured input in STT-2



CRIEPI

Difference of hydraulic head between KXTT3 R2 and other sections

Test #	Time (YYMMDDHHMMSS)	KXTT1 R2 (mH_2O)	KXTT2 R2 (mH_2O)	KXTT4 R3 (mH_2O)	KA3005A R3 (mH_2O)
PDT-2	970513110325	1.84	0.48	2.40	1.87
	970516110325	1.89	0.44	2.40	1.83
STT-1a	970704235732	6.11	1.31	7.11	6.46
	980127121024	11.06	3.10	12.90	11.82
STT-2	980605130722	4.09	0.37	5.82	5.06
	981010074320	2.93	-0.26	3.97	2.92

Estimation of STT-2 tracer tests

S McKenna (Sandia)

Estimation of the STT-2 Tracer Tests

Aspo Task Force Deliverable: Task 4F

Sean A. McKenna
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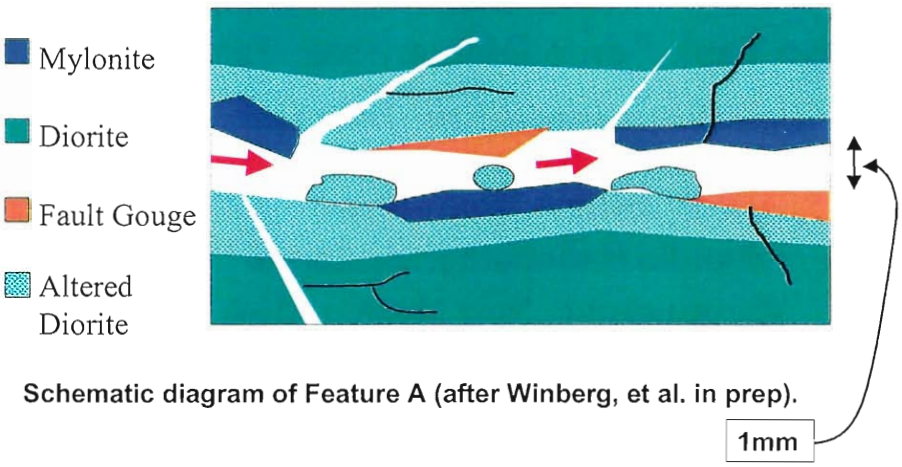
Albuquerque, New Mexico USA

Sandia National Laboratories

Objectives

- Employ multirate mass-transfer model to estimate breakthrough curves for STT-2 tracer tests
- Compare to STT-1 results
- Evidence of flow on two separate pathways

Multirate Conceptual Model



Schematic diagram of Feature A (after Winberg, et al. in prep).

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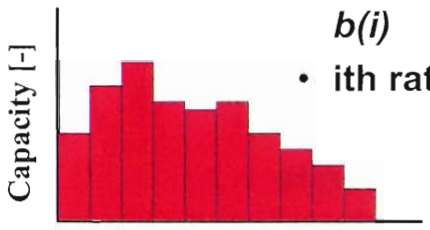
Multirate Distribution

- ith capacity = *b(i)*
- ith rate = $\alpha(i)$

$$\beta_{tot} = \sum_{i=1}^{N} b(i)$$



$$\mu = \frac{1}{N}\sum_{i=1}^{N} \log(\alpha(i)) \qquad \sigma = \sqrt{\frac{1}{N}\sum_{i=1}^{N} (\log(\alpha(i)) - \mu)}$$

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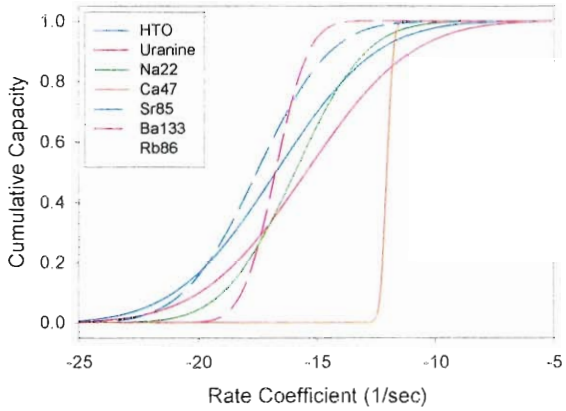
Lognormal Distributions



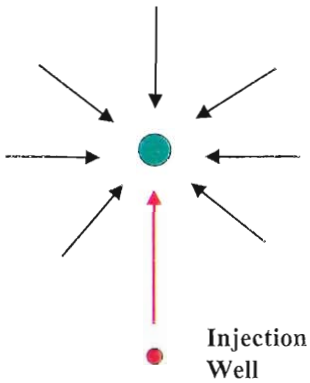
Example lognormal distributions of mass-transfer rate coefficients estimated for the STT-1 tracer test

Dilution Factor

- **Dilution factor**

$$Dilute = \frac{Q_p}{Q_{inj}}$$

$$Dilute = \frac{Q_p}{Q_{inj}} \frac{1}{RMF}$$



Background

- Estimation of STT-1 tracer tests at 400 ml/min pumping rate
- Blind prediction of STT-2 tracer tests
  - Reduced velocity and dilution factor due to 200 ml/min pumping rate
  - Additional tracers not used in STT-1
- Some STT-2 BTC's show effects of two pathways

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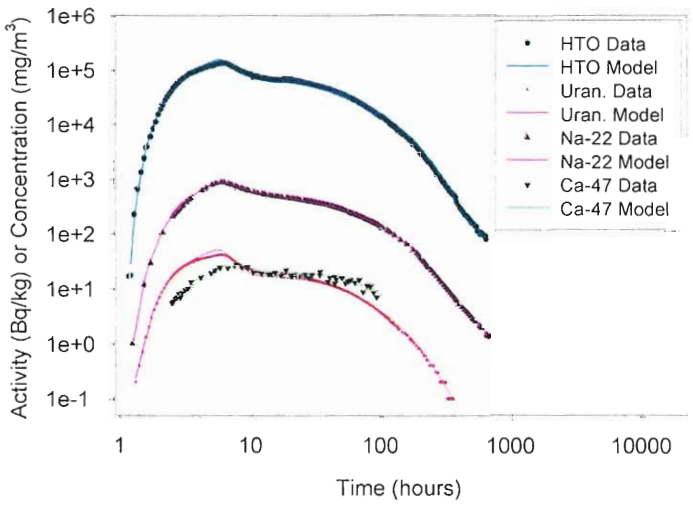
Example Estimation: STT-1



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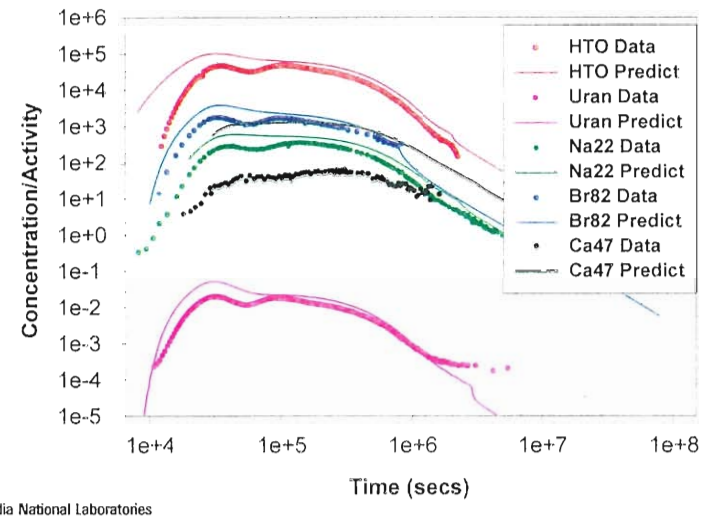
STT-2 Blind Predictions



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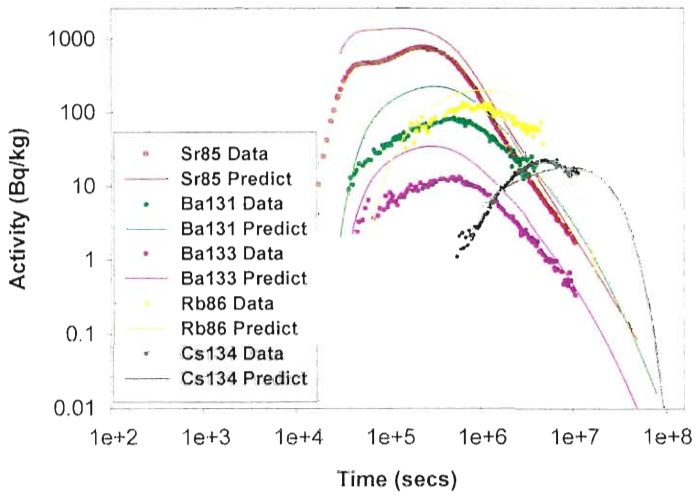
STT-2 Blind Predictions (cont.)



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Blind Prediction Summary

- All Predictions overestimated actual mass observed in BTC's
- First peak in BTC is poorly predicted, predictions of second peak and tail are closer to observed data
- Quality of predictions decreases with increasing sorption strenght

Single-Path Approach

- Try to estimate parameters with flow along a single pathway
- Estimate velocity, dilution factor and dispersion on HTO data then hold constant for all tracers
- Estimate three parameters independently for each tracer:
  - mean of multirate mass transfer distribution
  - standard deviation of m.m.t. distribution
  - total capacity of system

Estimated Flow Parameters

- Flow parameters estimated on HTO data and used for all tracers
- Velocity:
  - 6.621x10-4 m/s
- Dispersivity:
  - 0.789 meters (17 percent of travel distance)
- Dilution Factor:
  - 498.9
- Retardation fixed at 1.0 for all tracers!

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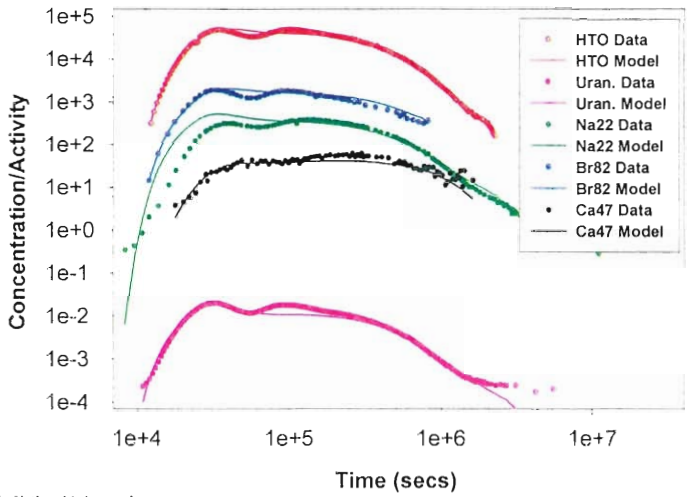
Single Path Estimations



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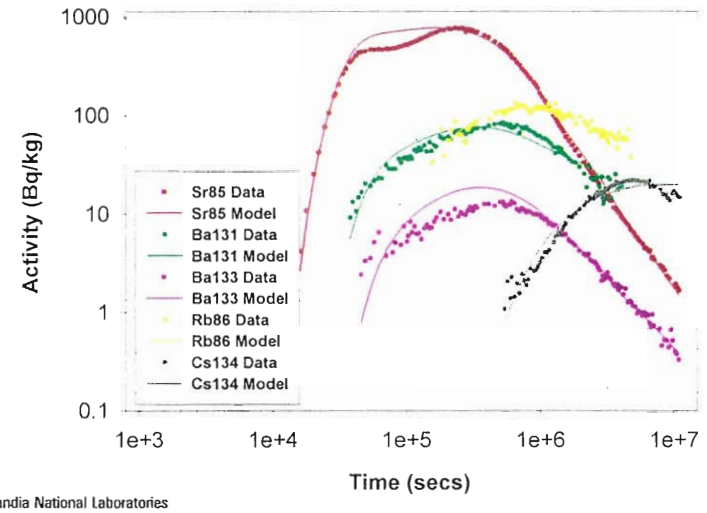
Single Path Estimations (cont.)



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Flow Parameter Comparison

- Less dilution in STT-2 than predicted from decrease in pumping rate
  - Greater proportion of flow in Feature A relative to STT-1
  - Decrease in injection rate versus STT-1
- Greater dispersion than seen in STT-1 estimations (0.79 vs. 6.0X10-05 meters)
  - Single path model; data from two pathways (?)
- Decreased velocity
  - Approximately 35 percent of STT-1 velocity

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Parameter Comparison

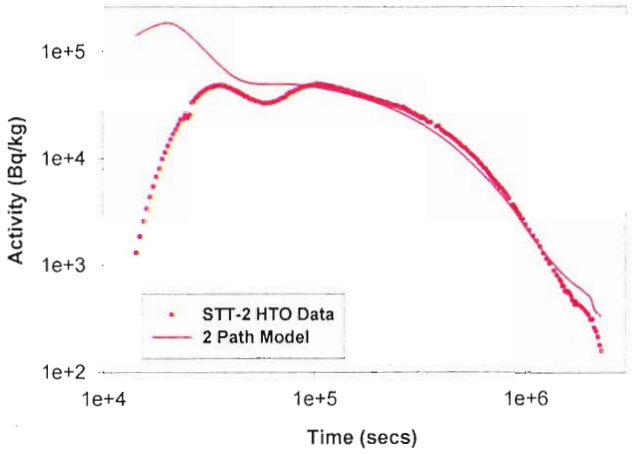
Tracer	STT-2 Predictions			STT-2 Estimations		
	β_{tot}	μ	σ	β_{tot}	μ	σ
HTO	77.4	-16.7	3.4	26.4	-13.2	1.6
Uranine	36.1	-15.4	3.5	136.6	-18.3	2.9
Na22	110.3	-15.9	2.38	195.1	-18.6	2.7
Br82	77.4	-16.7	3.35	1963.8	-21.8	2.4
Ca47	33.8	-12.0	0.22	71.7	-14.1	0.2
Sr85	286.4	-17.5	2.43	279.7	-18.1	2.5
Ba131	566.0	-16.7	1.11	477.0	-16.8	0.03
Ba133	566.0	-16.7	1.11	532.0	-16.8	0.7
Rb86	704.3	-16.0	0.09	709.0	-16.6	0.1
Cs134	2942.7	-17.6	0.032	3634.7	-18.3	0.02

Two-Path Estimation

- First approach:
  - independent velocity for each path
  - estimation of mass fraction in each path
  - same mass-transfer distribution for each path
- Second approach:
  - independent velocity in each path
  - estimation of mass-fraction in each path
  - independent mean and std. dev. of multirate distribution (same total capacity)

Two-Path Model

Independent Velocities, Single Mass Transfer Distribution



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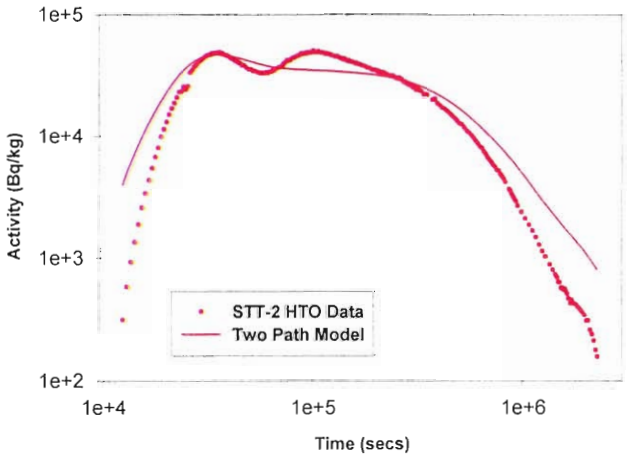
Two Path Model

Independent Velocities, Two Mass-Transfer Distributions



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Summary

- General shape and timing of STT-2 BTC's is predicted by blind prediction
- Single-path multirate model provides good fits to tail of BTC's, but unable to account for two-path advective behavior
- Flow parameters are significantly different from STT-1 estimations
- Transport parameters also differ from STT-1 estimates

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Task 4F2 Modelling

W Dershowitz, M Uchida and A Fox (JNC/Golder)

Executive Summary of Task 4F2 Modelling

JNC/Golder
W. Dershowitz, M. Uchida, A. Fox

31 January 2000

Approach

The JNC/Golder team predictions for Task 4F matched the breakthrough curves for sorbing and non-sorbing tracers too well: As a result, it is difficult to improve the model. Nevertheless, we have high confidence that the model that we have is *not* an accurate reflection of the transport pathways within "Feature A" – rather it is an indication that the extensive hydraulic and tracer testing which preceeded Task 4F was sufficient to produce a well-calibrated model.

The goal of Task 4F2 was to explore what minor changes could be made to our model to provide a better match. We did not explore alternative pathway models, since the model we have was the result of extensive calibration to previous site tracer tests. Rather, we adjusted minor parameters such as effective dispersion, diffusion, porosity, and pathway perimeter. This is supported by the fact that some of our predictions over-predicted recovery, and some under-predicted recovery, indicating that the errors are in geochemical properties along pathways, rather than a systematic error in the geometry of the pathways. Different tracers can, for example, experience different effective dispersion and diffusion along pathways even through they are following the exact same pathways, within the same flow field.

Analysis

We have chosen to look at a few tracers, which typify the type of errors which occurred in our predictions.

These tracers are:

- Uranine, for which the shape of the peak breakthrough was wrong. This might be improved by changing the relative strength of each of the pathways contributing to the breakthrough, or by adding pathways with specific properties;
- Cesium-135, for which our recovery was too low. This might be improved by decreasing matrix porosity and pathway perimeter;
- Rubidum-86, for which our recovery was too low and our peak somewhat delayed. This might be improved by reducing matrix porosity, pathway perimeter, sorption, and diffusion;
- Strontium-83, for which our recovery was too high. This might be improved by increasing matrix diffusion depth and pathway perimeter.

Results of these approaches are illustrated in Figures 1 through 4.

Conclusions

The modelling carried out for Task 4F2 was not very useful, since we did not really learn anything about the nature of flow and transport in Feature A. Rather, we learned the limitations of model calibration, and the number of variables which are available to match observed breakthrough curves.

1. The JNC/Golder Task 4F prediction was calibrated to the level possible without detailed understanding Because the forward model is confined to physical parameters and structures, there are limited degrees of freedom for model calibration and improvement. In order to improve the geochemical model fit, for example, it was necessary to add structural features to the model which had not been characterized by SKB.

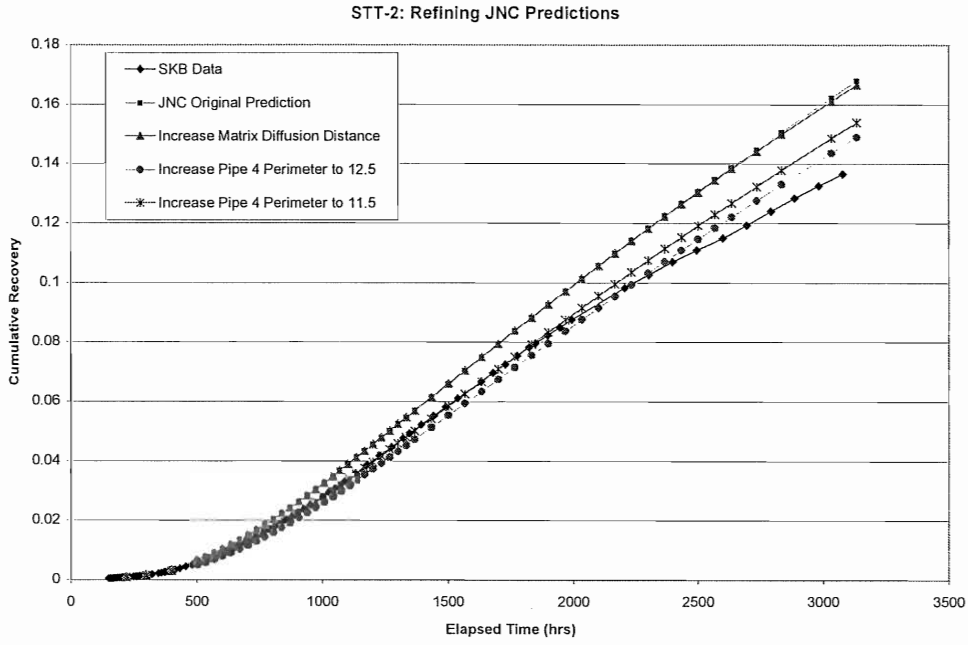

Figure 3: Decrease Matrix Porosity, Pipe Perimeter and Diffusion Depth to Improve Cesium Recovery

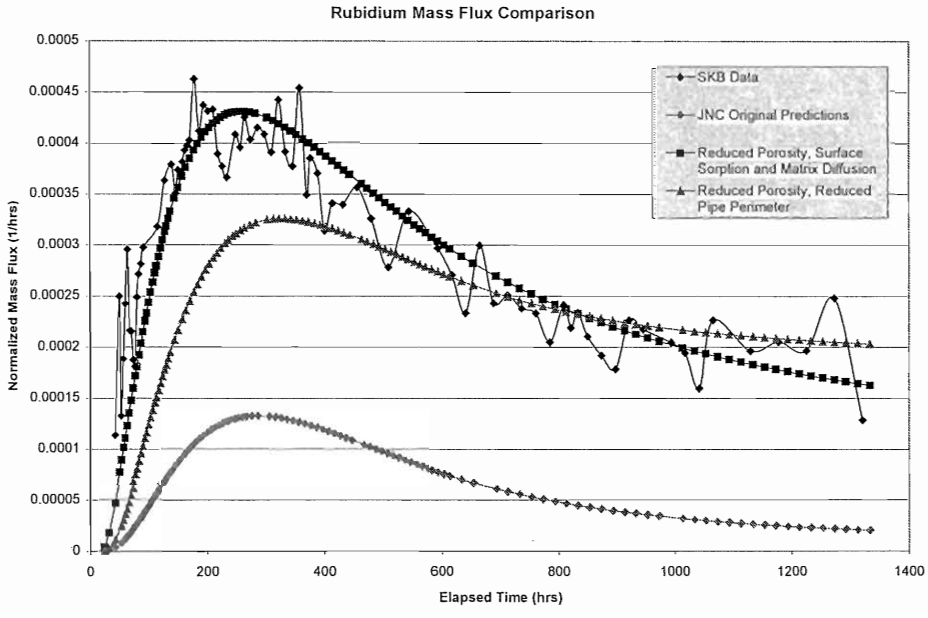

Figure 4: Decrease Matrix Porosity, Sorption, Diffusion to Depth Improve Rubidium Recovery

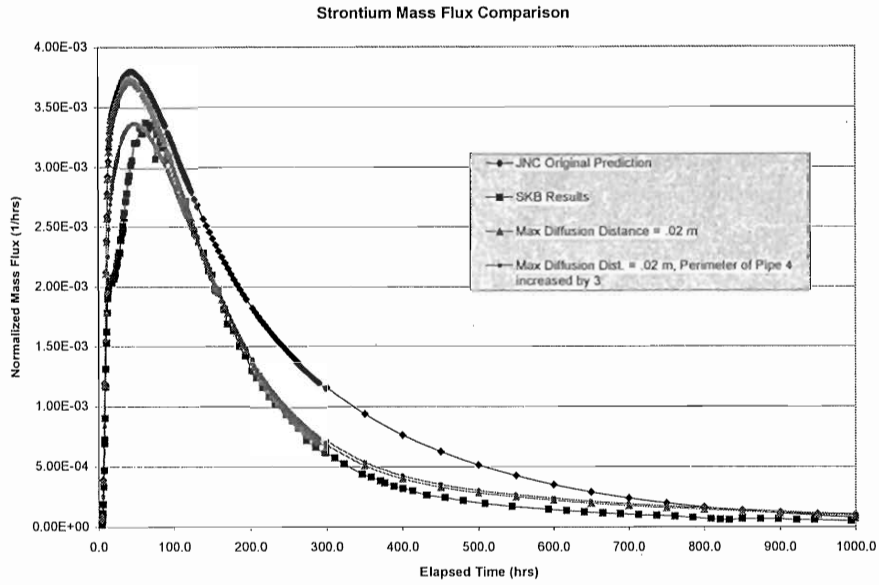

Figure 5: Increase Diffusion and Sorption to Decrease Strontium Recovery

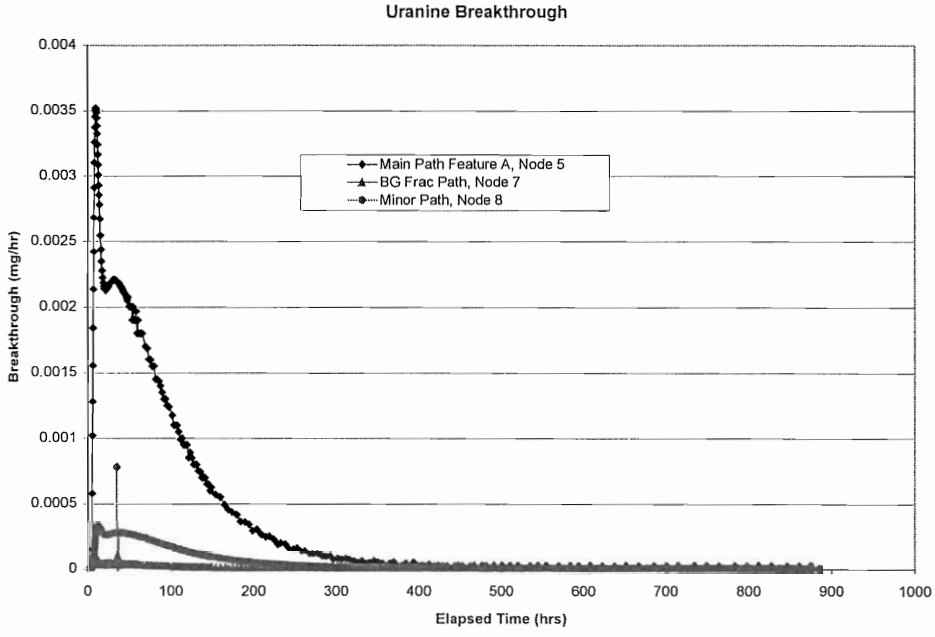

Figure 1: Contributions of Three Pathways to Uranine Breakthrough

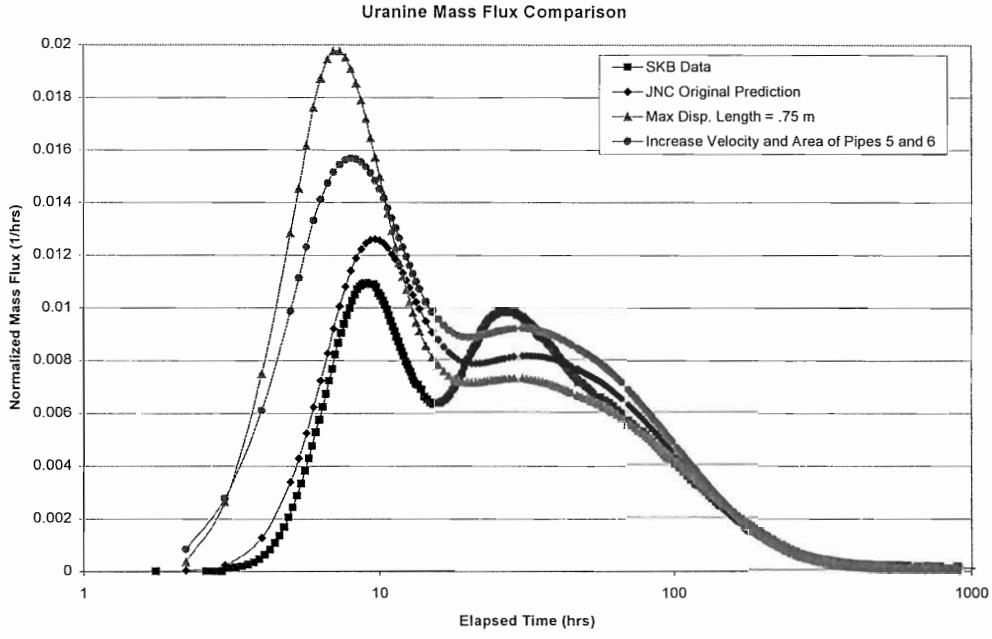

Figure 2: Adjusting Pathways and Diffusion to Improve Uranine Match

Conclusions from modelling Task 4E& F

A Jacob and W Heer (PSI)

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Conclusions from modelling Task 4e and 4f

Andreas Jakob, Walter Heer

Decision: Very simple model for flow and transport

- stay as simple as possible (system understanding)
- minimum number of parameters
- based on our experiences from the Grimsel modelling

Flow:

- streamtube concept
- homogeneous and isotropic transmissivity
- averaged, steady-state background flow-field
- constant injection and pumping flow-rates

Transport:

- dual-porosity-medium model (DPM), (continuum, deterministic)
- model calibration on uranine breakthrough PDT3 and PDT4 only
- interpreted values for D_P, K_a and K_d from laboratory measurements on Äspö diorit

↘ **fairly good predictions for all three tracer tests**

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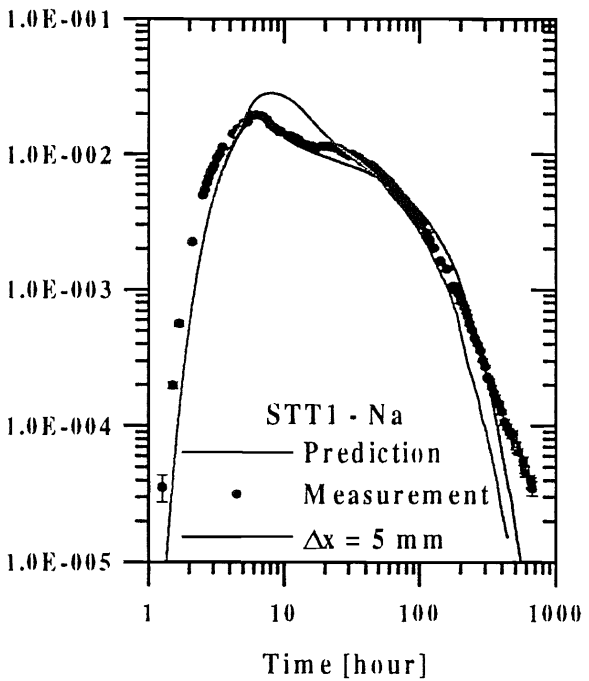
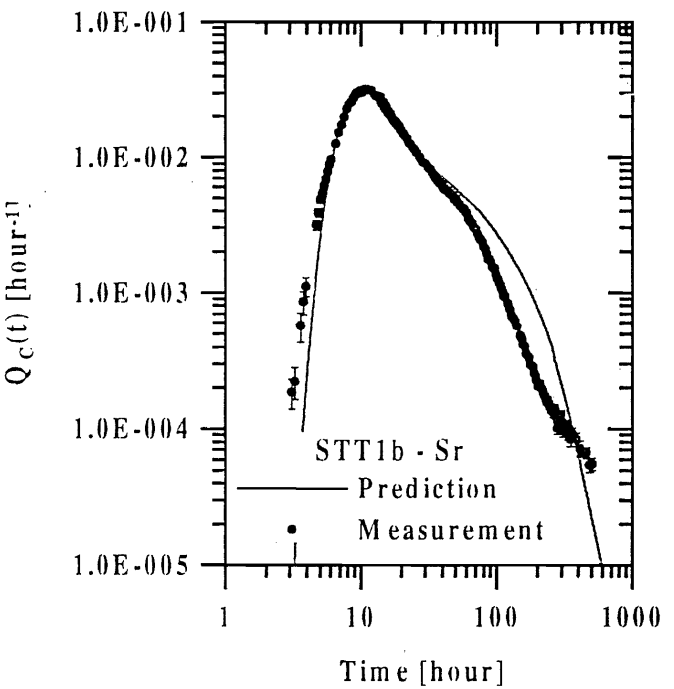
Blind-predictions

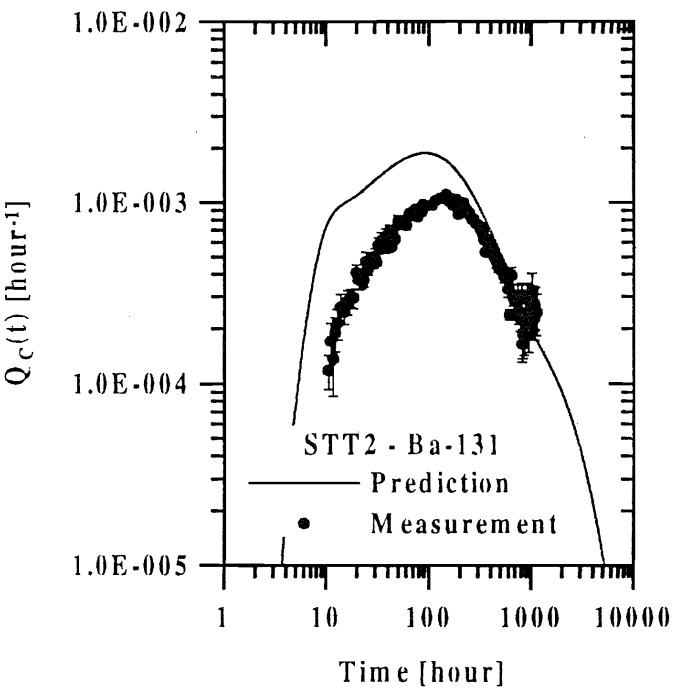
STT1



Stt1b



STT2



Reasons for the success

The experimental set-up was still quite "simple"

- Hydrology << Transport
- Heterogeneities (decimetre scale) play only a minor role

However, impact from geologists (and other scientists) was needed for an appropriate model structure

- at least two fracture families
- information on fracture mineralogy
- one-sided matrix diffusion into fault gouge and cataclasite
- values for the penetration depth ($\Delta x \cong 5$ mm)
- values for the porosity of fault gouge ($\varepsilon_P \cong 15$ %) and cataclasite ($\varepsilon_P \cong 3$ %

Laboratory data for the transport parameters could be applied

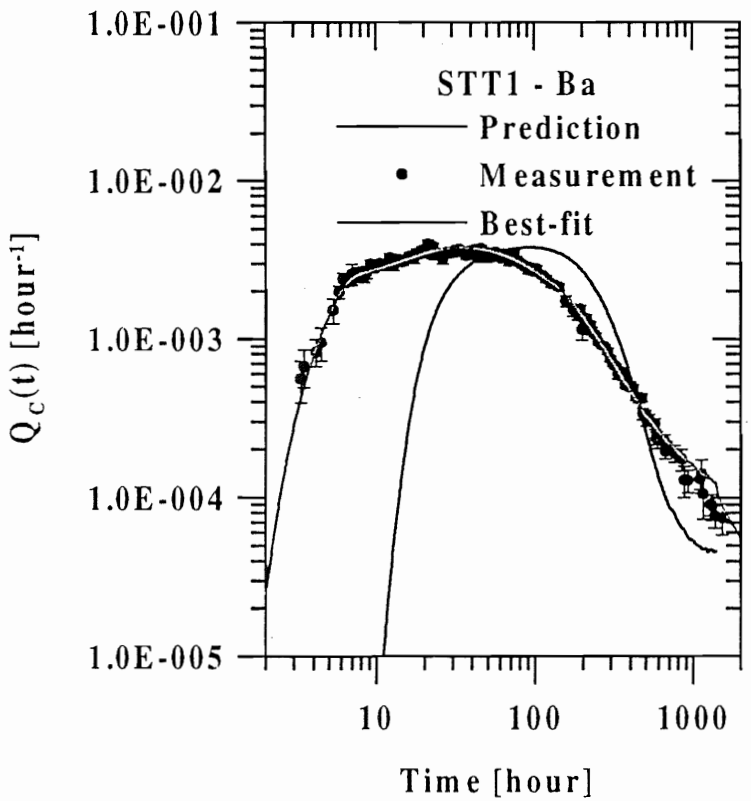
- but they had to be interpreted (re-scaled) and
- these values were good enough for the predictions

The DPM-model accounts for the most important transport mechanisms

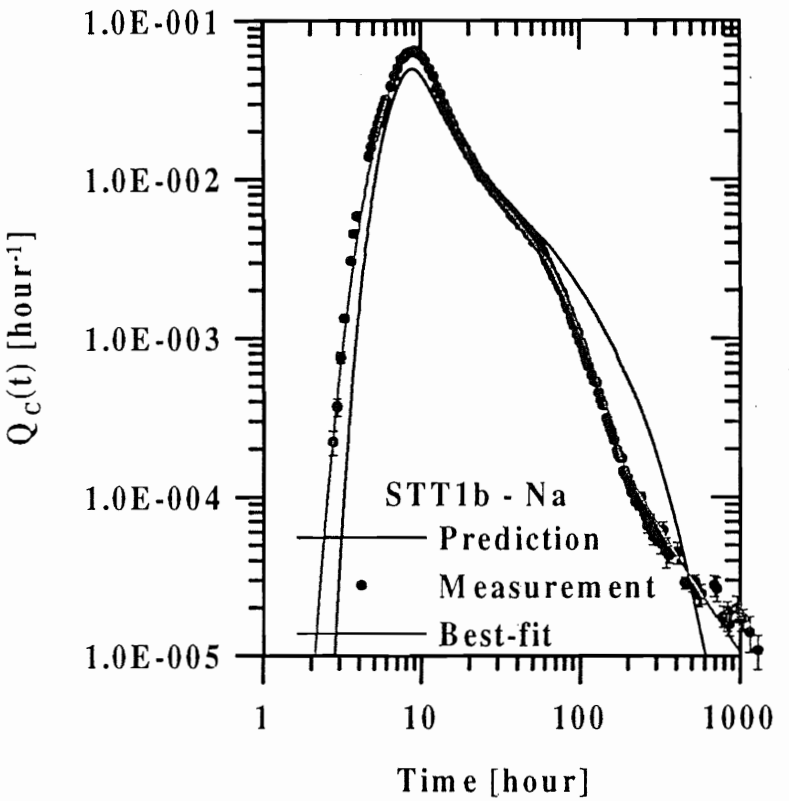
- simple but versatile and "understandable" model
- a few (lumped) transport parameters (no fudge-factors)
- no further transport mechanism was needed

Best-Fits

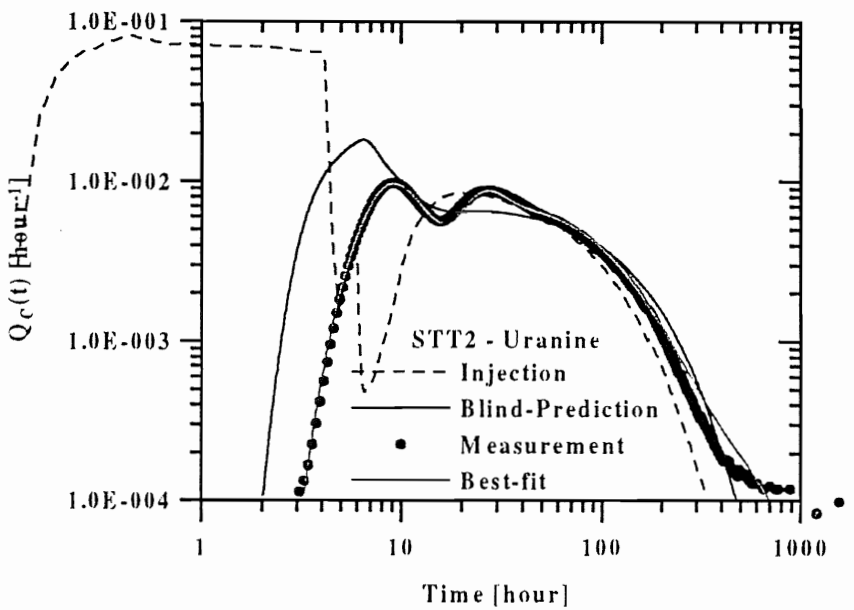
STT1

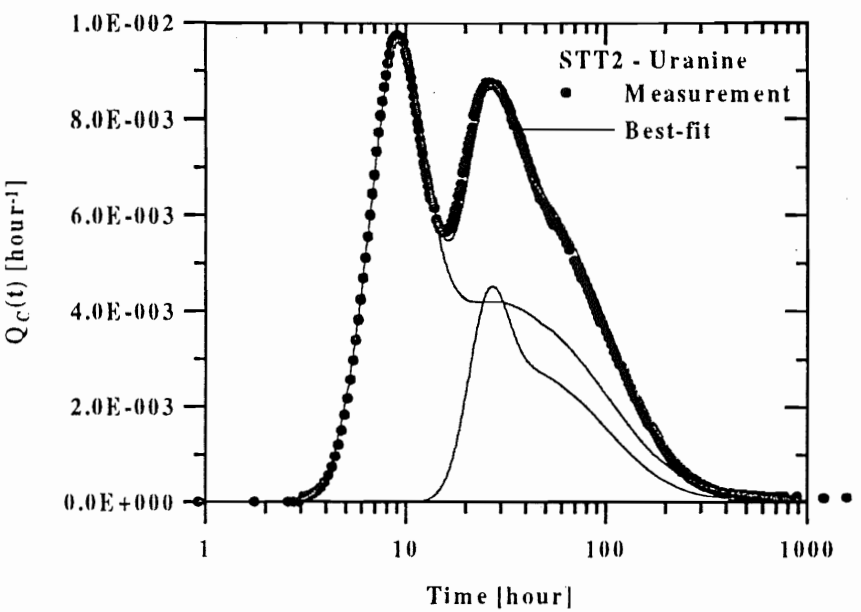


Stt1b

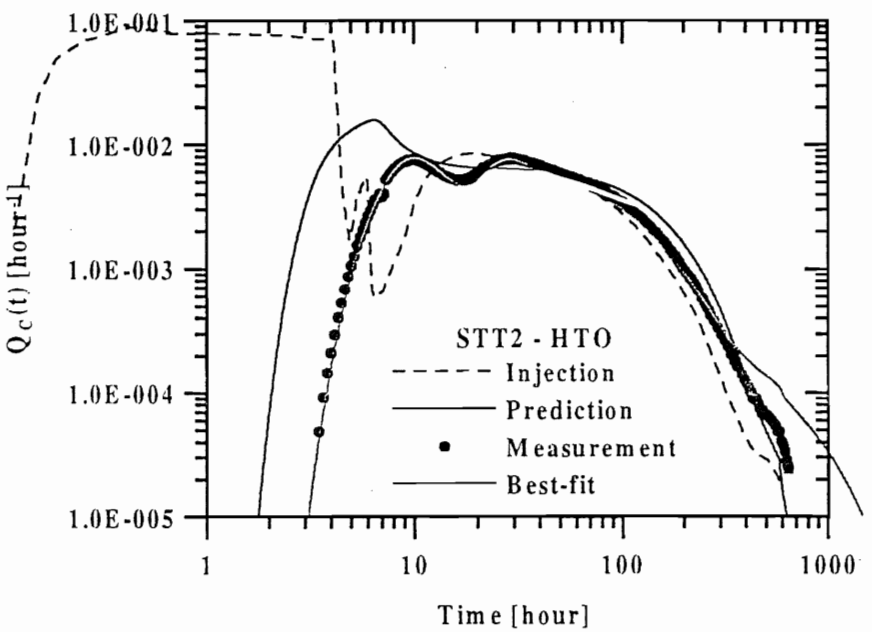


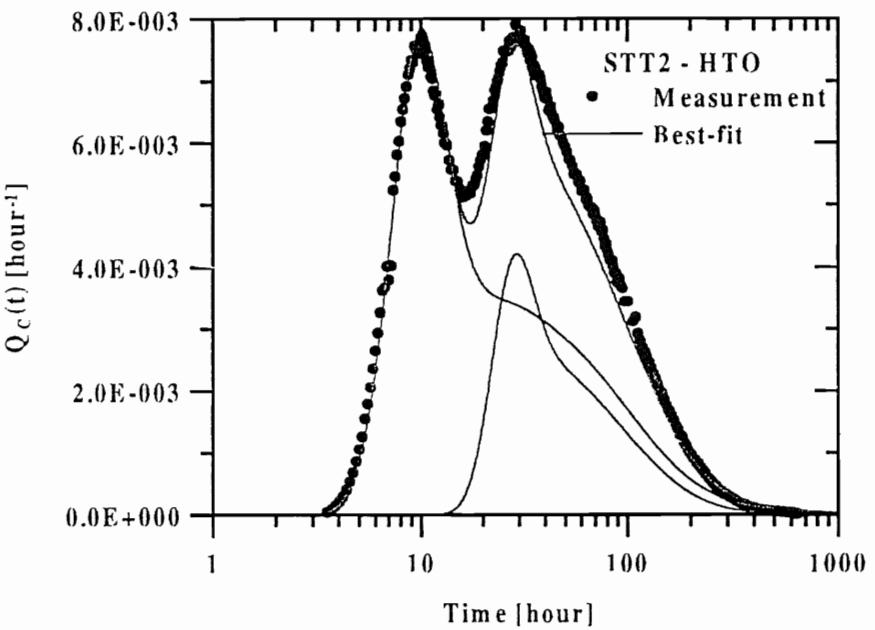
Conservative tracer uranine



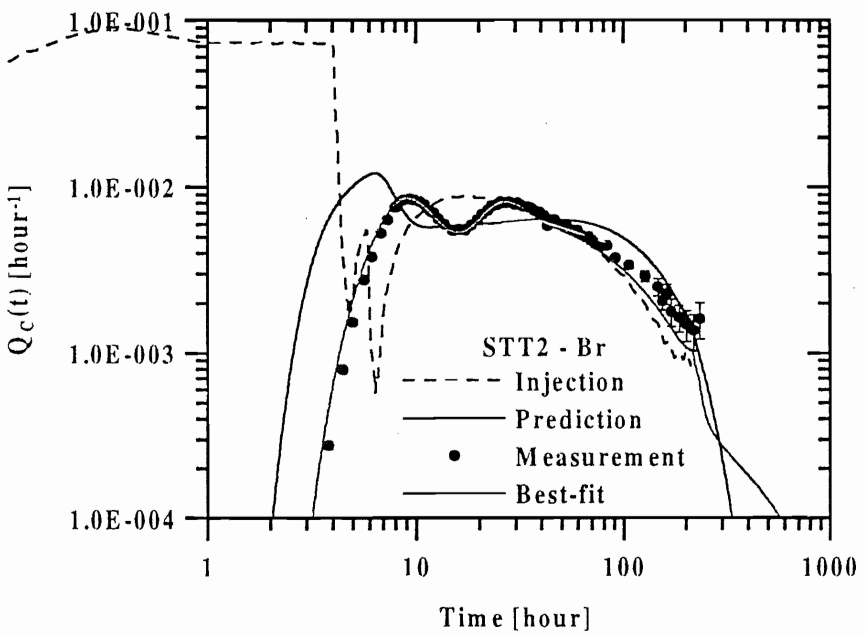


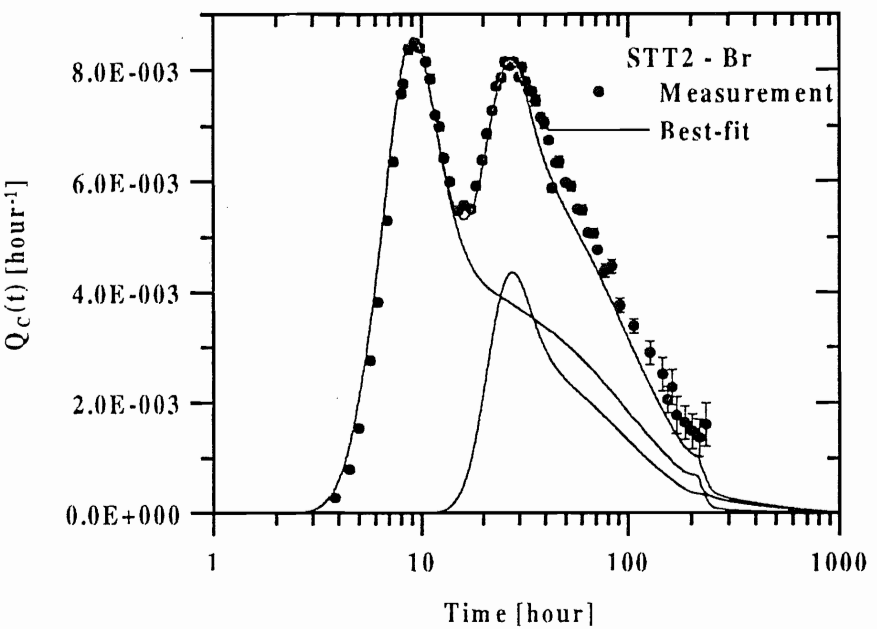
Conservative tracer HTO



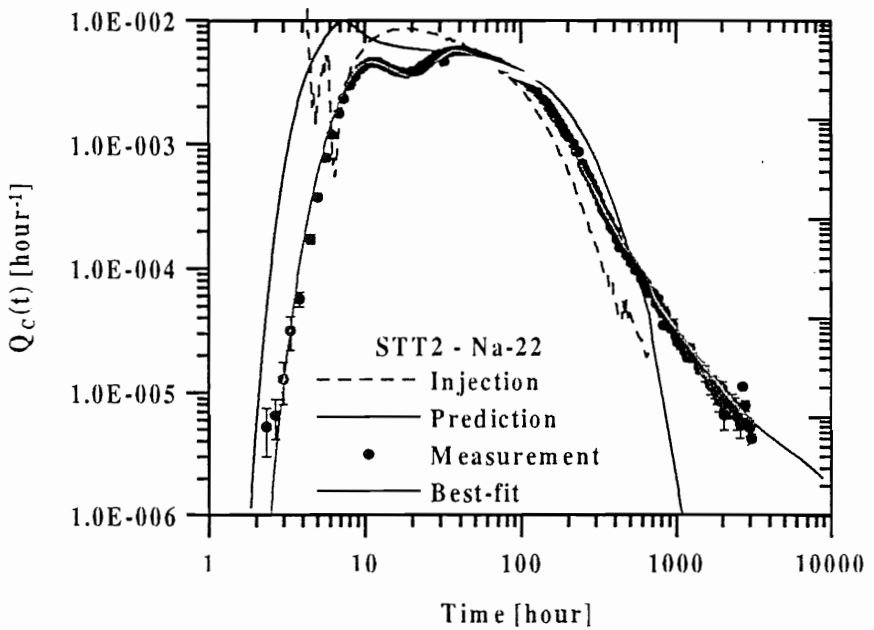


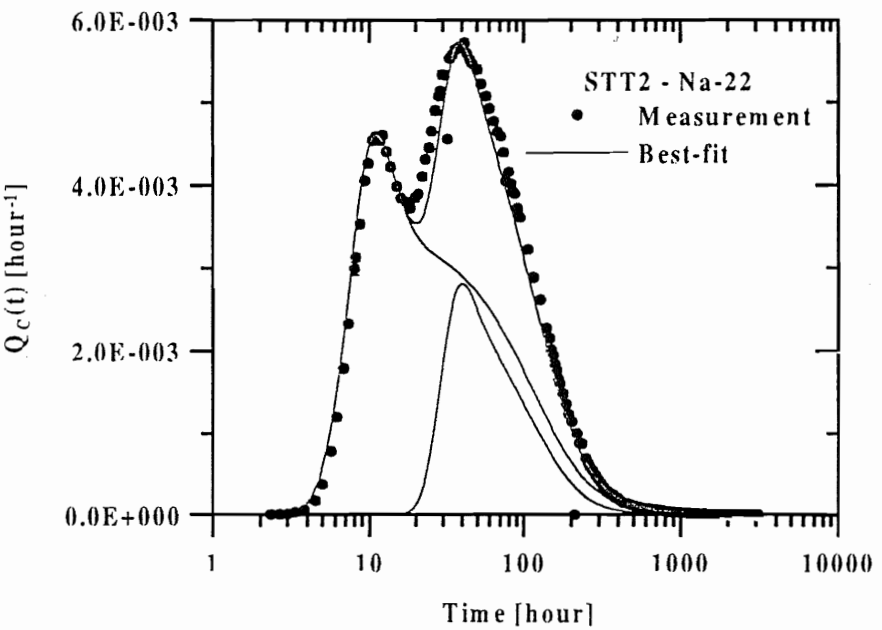
Conservative tracer bromine



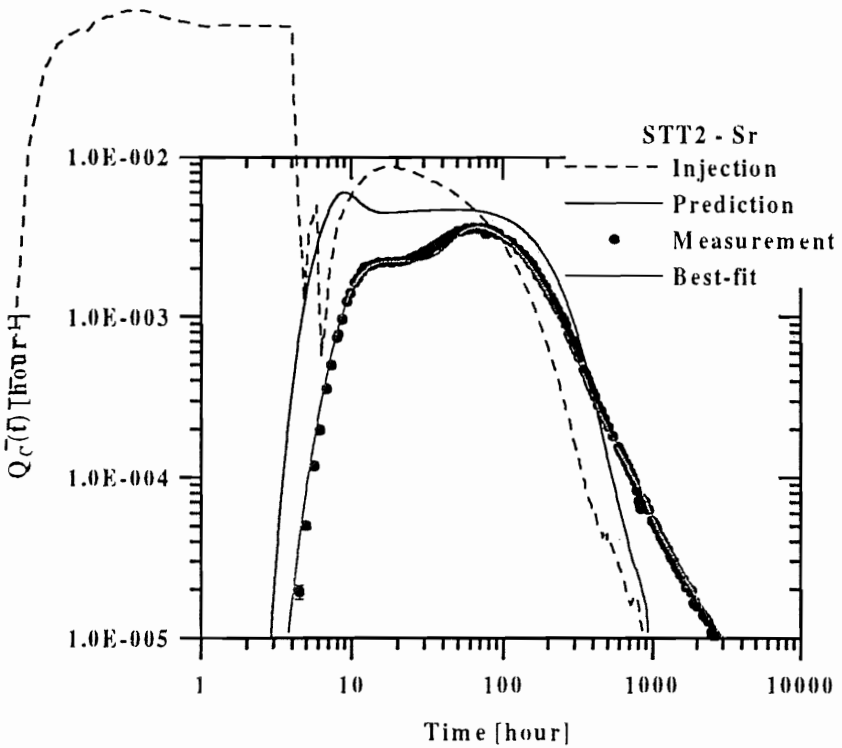


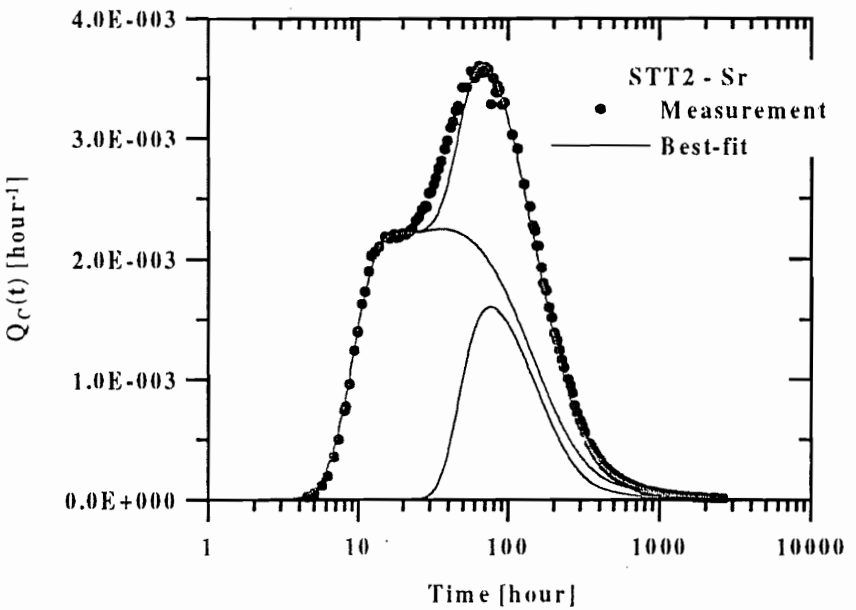
Conservative tracer sodium



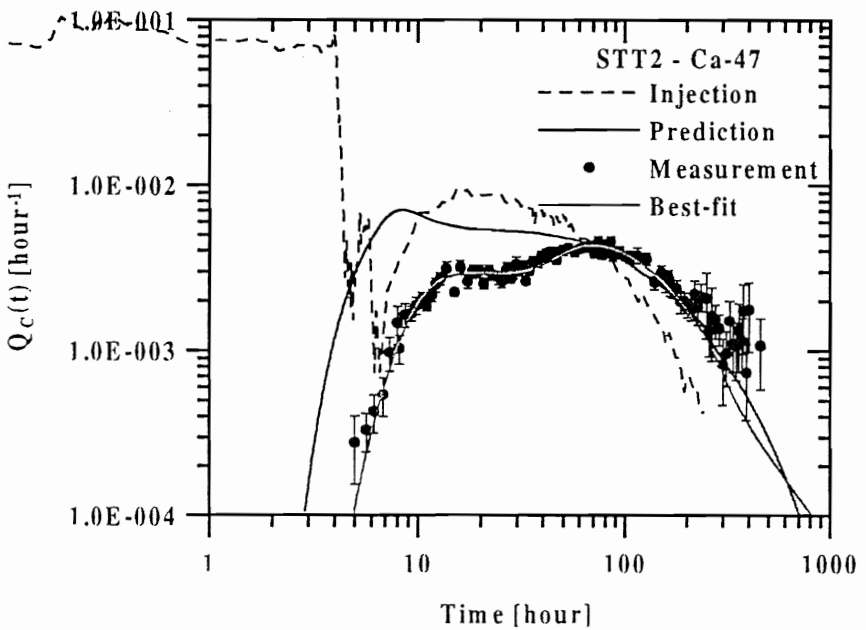


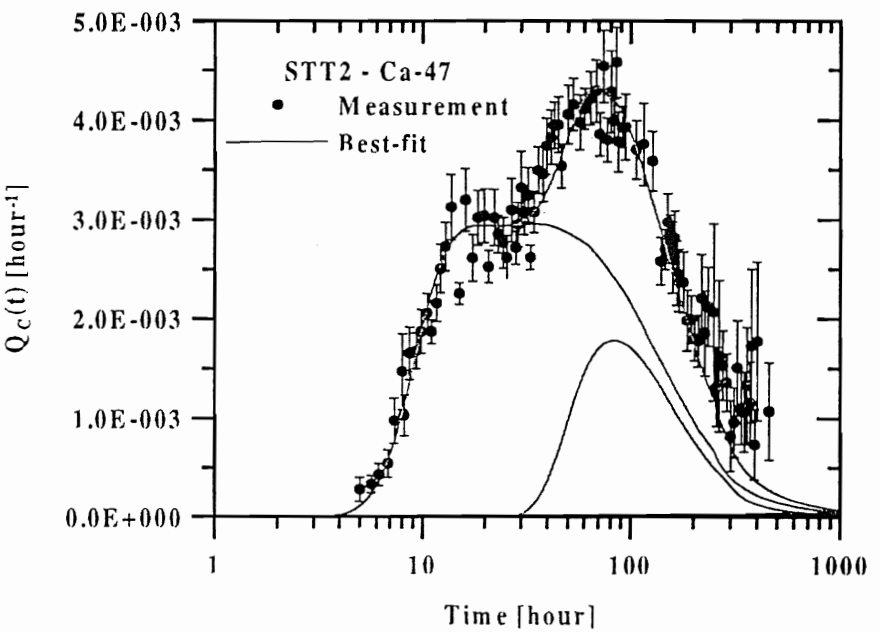
Weakly sorbing tracer strontium



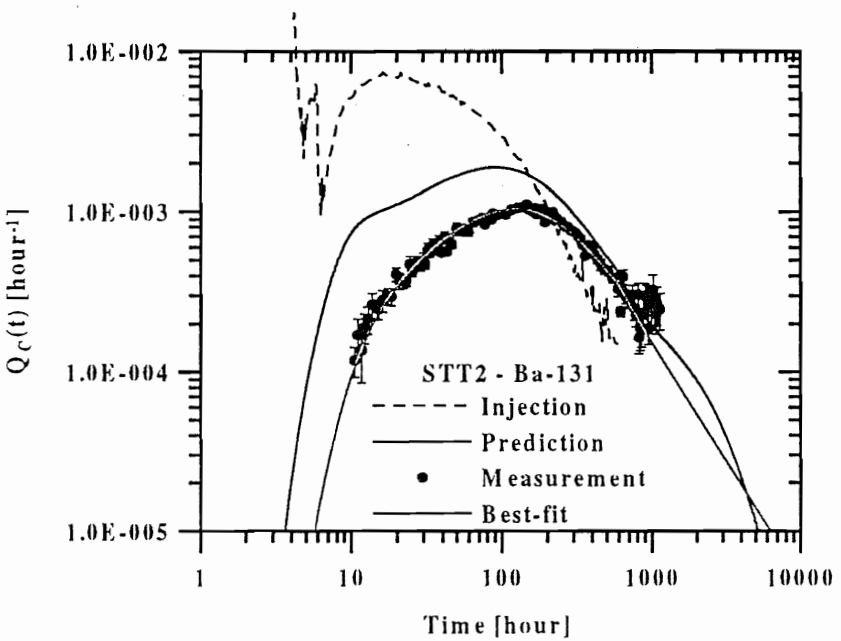


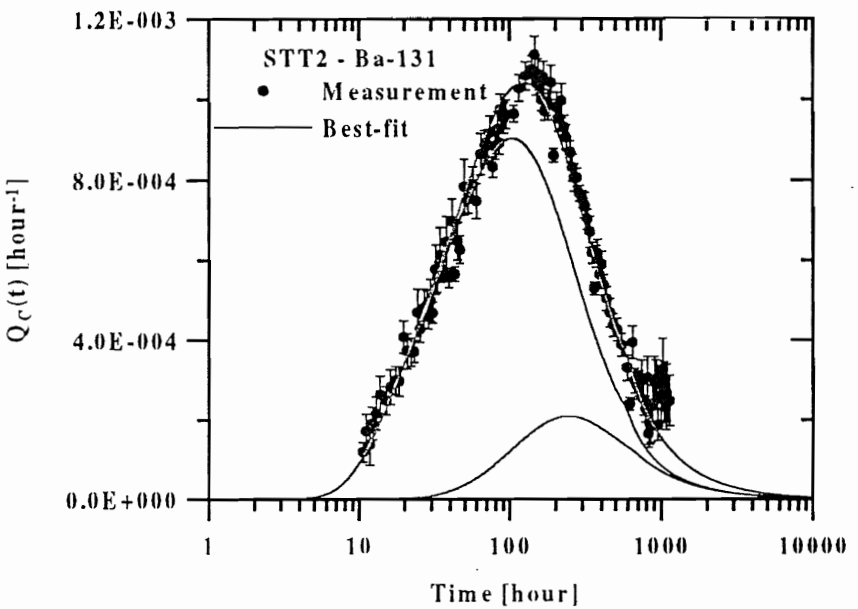
Moderately sorbing tracer calcium



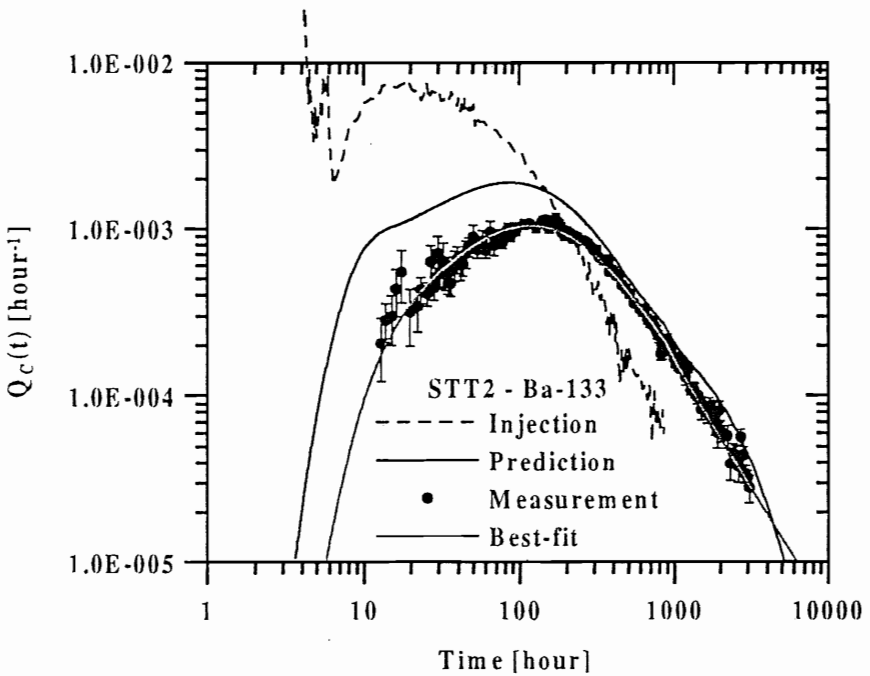


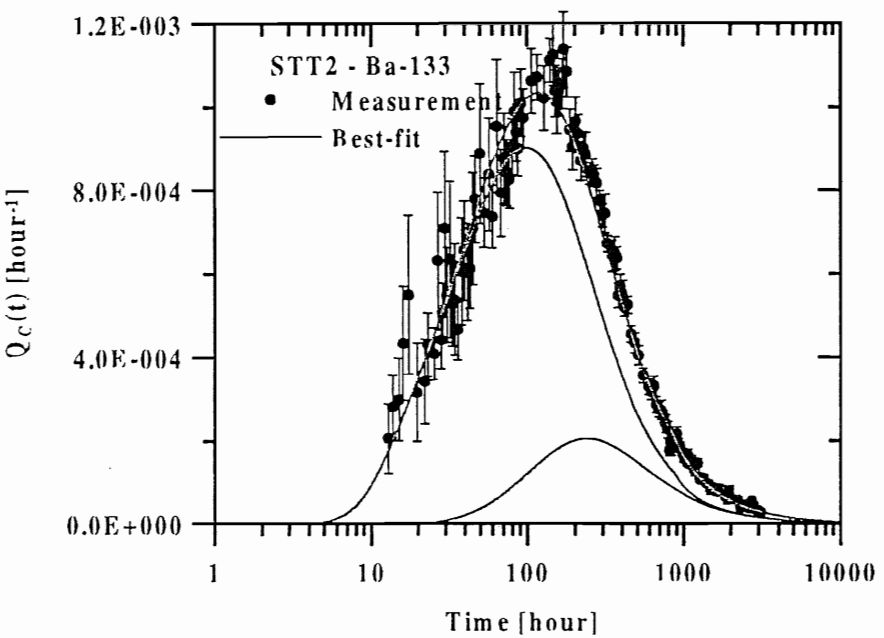
Stronger sorbing tracer barium-131



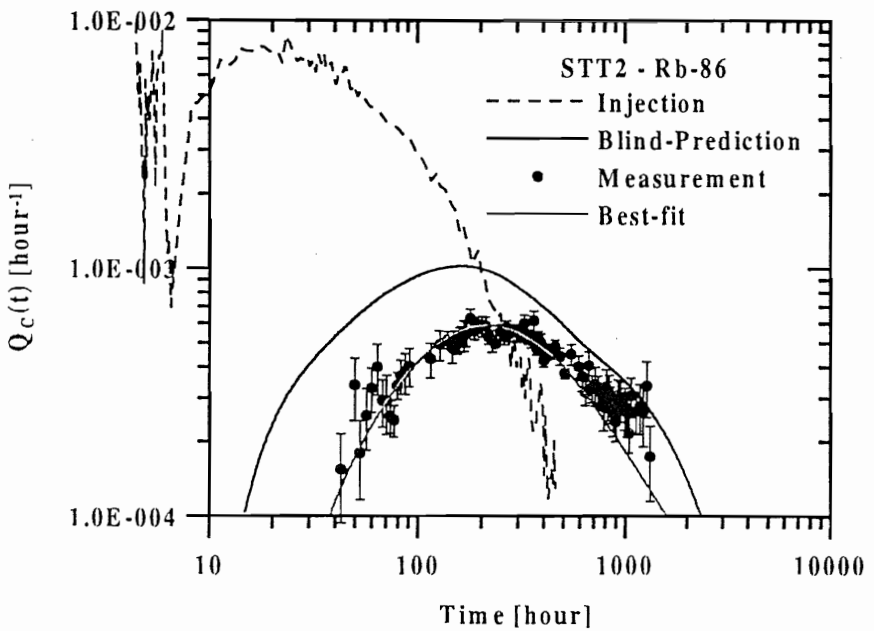


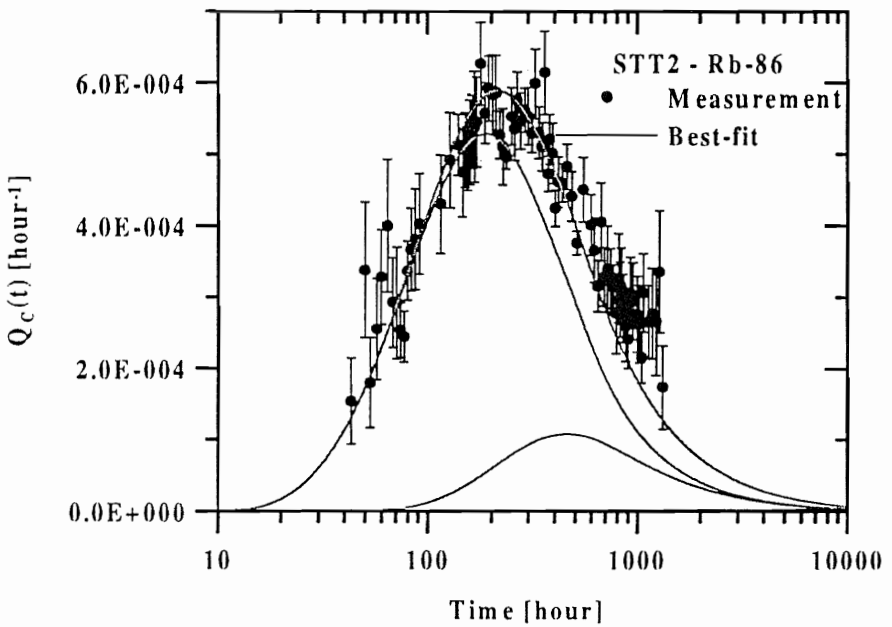
Stronger sorbing barium-133



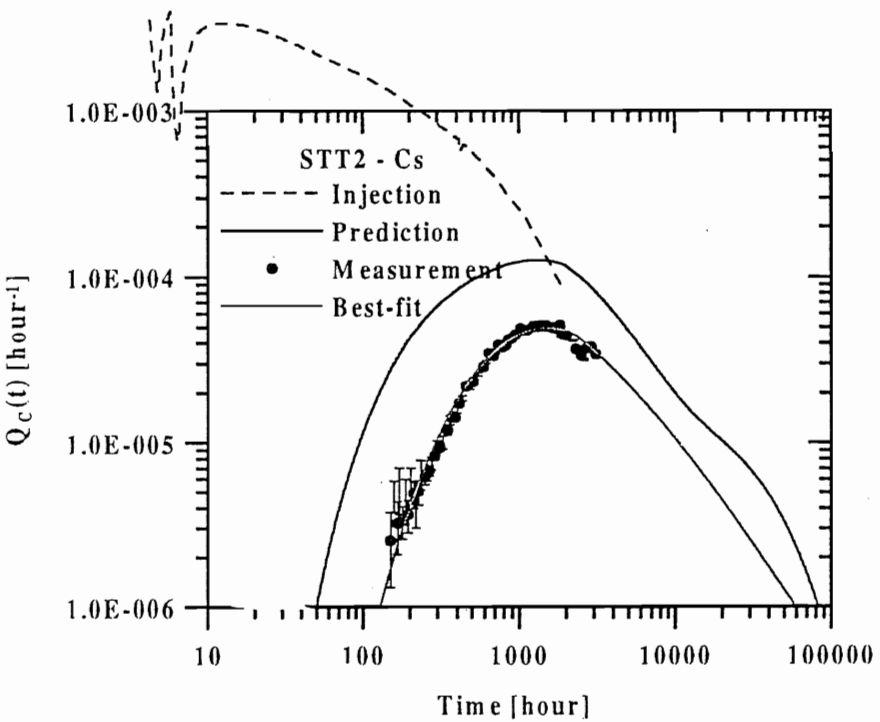


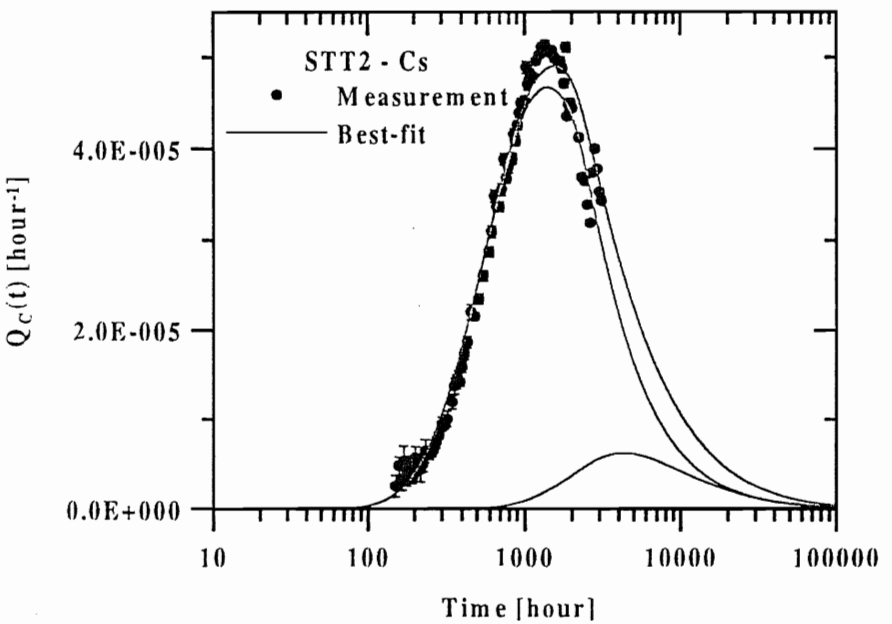
Stronger sorbing tracer rubidium





Stronger sorbing tracer caesium





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Results from inverse modelling of the tracer breakthrough curves

- no serious limitation of the model could be detected
- for STT1 and STT2 two (independent) fracture families were required
- for STT1b: the first fracture family was sufficient
- values for the transport parameters may differ from laboratory data by an order of magnitude
- hence, they should be measured on fault gouge and cataclasite originating from feature A
- these best-fit data are consistent
- no further transport mechanism could be observed
- for caesium a significant tracer loss (50, 30%) had to be assumed twice
- unfortunately, important information on nuclide/rock interaction was covered by the second part of the injection distribution

The PSI modelling-team has learnt a lot

- increased confidence in our methodology and models
- such exercises are highly appreciated
- however, ...
    - more complex systems with much stronger interaction of hydrology and transport
    - larger travel distances
    - a final tracer test using actinides for demonstration purposes only?

Final evaluation of TRUE-1 tests

V Cvetkovic and H Cheng (KTH), J-O Selroos (SKB)

Evaluation of Sorbing Tracer Tests STT-1 and STT-1B in the First TRUE Stage

TASK 4E

Based on
TRUE-1 Final Report of the First Stage of the Tracer Retention Understanding Experiments (Winberg (ed.), in prep.)

TRUE MODELLING TEAM:
Vladimir Cvetkovic, Water Resources Eng., KTH
Hua Cheng, Water Resources Eng., KTH
Jan-Olof Selroos, SKB
April 1999

EXECUTIVE SUMMARY

We evaluated and interpreted the BTC-data for the sorbing tracers tests STT-1 and STT-1B using the LSAR framework (Cvetkovic et al. 1999). The observed BTCs for sorbing tracers exhibit significant kinetic effects, in particular for more strongly sorbing tracers; these are attributed to diffusion and sorption in the rock matrix, and to sorption in gouge material. It appears that the retention observed in the field cannot be predicted based on the laboratory data for κ alone. Calibration with a factor f, as well as with parameters K_d^g and α for gouge, was required for obtaining a close comparison between the modelled and observed BTCs. The calibration parameters f and K_d^g vary only mildly between different tracers, and for the different TRUE-1 tests.

INTRODUCTION

Predictions of breakthrough curves (BTCs) for sorbing tracers of STT-1 and STT-1B deviate from the experimental data. The objective of this evaluation is to provide a consistent interpretation of the measured BTCs with a minimum set of calibrated field-scale parameters. A comprehensive description of the theory, evaluation procedure and results is given in Cvetkovic et al. (in preparation).

STT-1 is performed in Feature A between boreholes KXTT4 R3 and KXTT3 R2 with a injection flow rate 400 ml/min, while STT-1B is also performed in Feature A, but between boreholes KXTT1 R2 and KXTT3 R2 with the same flow rate 400 ml/min.

Feature A is perceived as a planar fracture with a spatially variable aperture. A tracer injected in a borehole within feature A is advected and dispersed, and is subject to various mass transfer reactions. In particular, a tracer diffuses into the rock matrix and (if reactive) sorbs on internal surfaces of the rock; gouge (infill) material may be present and enhance sorption, i.e. retention.

EVALUATION FRAMEWORK

The Lagrangian stochastic advection-reaction (here abbreviated as LSAR) framework for reactive transport in rock fractures (Cvetkovic et al., 1999) is employed for the evaluation.

Solving the system of coupled transport equations for a single trajectory, a new parameter, β, was derived; β is a random quantity integrating the velocity-weighted variable aperture along a flow path. β controls surface sorption and diffusion/sorption into the rock matrix, and is related to the flow field. This result enables us to directly account for the effect of flow heterogeneity on the mass transfer reactions. The sorption in the gauge material is assumed to be a first-order kinetically controlled reaction, which is not influenced by β.

All mass transfer reactions considered in Cvetkovic et al. (1999) are assumed linear whereby the coupled effect is obtained by convolution. In particular, solutions for

individual mass transfer processes for pulse injection are convoluted with the input (tracer discharge vs time) in the injection borehole. To account for dispersive effects, the convoluted result for a single flow path is integrated over different flow paths described by a distribution of τ and β . τ and β have been shown to be significantly correlated both for generic conditions (Cvetkovic et al., 1999), and also for the flow conditions of feature A (Cvetkovic et al., in preparation). Based on these results, we establish an approximate linear (deterministic) relationship between τ and β using Monte Carlo simulations.

The water residence time distribution $g(\tau)$ (that accounts for dispersion effects due to advection variability) is contained in the breakthrough curves (BTCs) of HTO and Uranine, and is obtained through deconvolution of the measured HTO BTC.

KEY PARAMETERS

The two key parameter groups, which control sorption and diffusion following Cvetkovic et al. (1999), are $K_a\beta$ for surface sorption, and $\beta\,\kappa$ for diffusion/sorption in the rock matrix. The parameter K_a and the parameter group κ have been determined in the laboratory for all tracers. The quantities τ (water residence time) and β are dependent on the flow conditions in the field and by definition cannot be determined in the laboratory.

Since measured BTCs indicate strong kinetic effects attributed to diffusion, we anticipate a comparatively small effect of surface sorption; hence we shall assume that the laboratory value of K_a is applicable in the field.

$\kappa = \theta[D(1+K_d^m)]^{1/2} = \theta(DR_m)^{1/2}$ where θ is the porosity of the rock matrix (note that we do not distinguish the "total porosity" from the "diffusion porosity"), D is the pore diffusivity in the rock matrix (θD is the effective diffusion coefficient in the rock matrix), and K_d^m is the sorption coefficient in the rock matrix. We found that κ, as determined in the laboratory, may not be applicable under field conditions. In other words, calibration may be required for the field-scale value. We define the field-scale κ as $f\kappa$, where $f>1$ is the *enhanced diffusion factor* to be calibrated on the BTC data. Using $\beta = k\,\tau$, we can write the parameter group controlling matrix diffusion/sorption as $f\,k\,\tau\,\theta(DR_m)^{1/2}$.

Two additional parameters to be considered in the evaluation are the distribution coefficient for the gouge K_d^g (once equilibrium is reached) and the kinetic rate (i.e. backward rate coefficient) α. The parameters K_d^g and α need to be inferred entirely from the measured BTC data since laboratory values are not available.

EVALUATION PROCEDURE

The evaluation procedure consists essentially of two steps:

1. We determine the water residence time distribution $g(\tau)$ by deconvoluting the HTO BTCs, accounting for diffusion into the matrix; the actual form of $g(\tau)$ is

assumed as inverse-gaussian, and the first two water residence time moments are calibrated.

2. We use $g(\tau)$ to model the reactive tracer BTCs by accounting for mass transfer processes, with parameters determined in the laboratory. If the modelled BTCs deviate from the observed BTCs, we enhance mass transfer by increasing the diffusion factor f (where $f\kappa$ is the calibrated value), and add sorption in gouge material.

Increasing κ by a factor f can imply larger values of the physical parameters (θ and D) and/or of the sorption coefficient K_d^m. If the calibrated value $f>1$ is due primarily to the physical factors, then f should be approximately constant for all tracers, irrespective of tracer sorption properties. If the calibrated value $f>1$ is primarily due to enhanced sorption properties (i.e. larger K_d^m in the field than measured in the laboratory), then f should be strongly dependent on tracer sorption properties. Furthermore, if $f>1$ is due to physical factors, then its impact has to be accounted for in the modelling of HTO BTCs. In other words, the above two steps become an iterative procedure, by which the moments of $g(\tau)$ are calibrated.

EVALUATION RESULTS

The BTC-data for TRUE-1 tests normalised with the total injected mass indicate that the sorptive tracers can be roughly classified into three groups: the weakly sorbing tracers Na and Sr, moderately sorbing tracers Ba and Rb, and strongly sorbing tracer Cs. The modelled BTCs for Na and Sr are more strongly influenced by the detailed form of the HTO BTC in comparison to the modelled BTCs for Ba, Rb and Cs.

The laboratory parameters and the field-scale parameters calibrated on measured BTCs are summarised in Tables 1 and 2 below. The calibrated temporal moments for HTO are mean=7h and variance=49h^2 for STT-1 and mean=5h and variance=1.5h^2 for STT-1B.

Tracer	K_a [m]	K_d^m [$m^3 kg^{-1}$]	D [m^2h^{-1}]	D_w [m^2h^{-1}]	$\kappa=\theta(DR_m)^{1/2}$ [$mh^{-1/2}$]
HTO	0.0	0.0	1.1E-7	8.4E-6	0.130E-5
Na	7.0E-7	1.4E-6	5.8E--8	4.8E-6	0.134E-5
Sr	8.0E-6	4.7E-6	3.6E-8	2.8E-6	0.155E-5
Ba	2.0E-4	2.0E-4	3.6E-8	3.0E-6	0.883E-5
Rb	5.0E-4	4.0E-4	9.0E-8	7.3E-6	1.968E-5
Cs	8.0E-3	6.0E-3	9.0E-8	7.3E-6	7.622E-5

Table 1: Laboratory parameters for HTO and sorbing tracers of the TRUE-1 tests. The parameters are defined in the Appendix. Additional laboratory values used in the evaluation are $\theta=0.004$ and $\rho=2700kg/m^3$.

Tracer	Enhanced diffusion factor f		K_d^g [-] for gouge (α=0.3h^{-1})	
	STT-1	STT-1B	STT-1	STT-1B
HTO	40	32	-	-
Na-22	40	32	1.0	0.5
Sr-85	40	32	2.0	1.6
Ba-133	40	-	4.0	-
Rb-86	45	34	5.0	4.0
Cs-137	50	-	10.0	-

Table 2: Calibrated parameters for HTO and sorbing tracers of the TRUE-1 tests; note that only the tracers for which laboratory data is available within the TRUE programme are included. The slope of the linear relationship $\beta = k\,\tau$ is k=3400 m^{-1} .

REFERENCES

Cvetkovic, V., J.O. Selroos and H. Cheng, Transport of reactive solute in single fractures, *J. Fluid Mech.*, **318**, 335-356, 1999.

Cvetkovic, V., H. Cheng and J.O. Selroos, Evaluation of TRUE-1 sorbing tracer experiments at Äspö: Theory and applications, SKB International Cooperation Report (in preparation).

Prediction of Sorbing Tracer Tests STT-2

in the First TRUE Stage

TASK 4F

TRUE MODELLING TEAM:
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Hua Cheng, Water Resources Eng., KTH
Jan-Olof Selroos, SKB
April 1999

Introduction

STT-2 was performed in the same path as in STT-1, but with a lower pumping rate of 200 ml/min. The tracers are injected in the borehole KXTT4 R3 and extracted in the borehole KXTT3 R2. The tracers used in STT-2 test are two conservative tracers (tratiated water and Br^{82}), and seven sorbing tracers (Na^{22}, Ca^{47}, Sr^{85}, Ba^{131}, Ba^{133}, Rb^{86} and Cs^{134}).

The injection section volume used is 1898 ml.

Conceptual and Mathematical Models

The same framework and models as in the evaluation of STT-1 and STT-1B are used.

The water residence time distribution $g(\tau)$ is assumed to have an inverse-Gaussian distribution. The moments of $g(\tau)$ are obtained by calibrating the calculated breakthrough against the experimental data from PDT2.

From the evaluation of STT-1, we found that the matrix diffusion needs to be increased by a factor f in order to explain the measured data, we also found the sorption in the gauge material may exist (Cvetkovic et al, 1999). STT-2 is performed in the same configuration as STT-1. Then the same factor f and parameters for the kinetic sorption in the gauge material from the evaluation of STT-1 are used for the prediction of STT-2. All other relevant parameters are laboratory values.

Flow and nonreactive Transport Results

Head value:

Tracer test Borehole section	$s_{(5\%)}{}^{c}$	$s_{(50\%)}{}^{c}$	$s_{(95\%)}{}^{c}$ (m)
***Q*=0.2 l/min**			
KXTT1	-62.7	-50.8	-47.7
KXTT2	-51.2	-47.5	-46.7
KXTT3	-48.2	-46.7	-46.4
KXTT4	-46.9	-46.5	-46.4
KA3005	-49.7	-47.6	-47.1

Sorbing Transport Results

The following tracer data has been used:

Tracer	K_a (m)	K_d (m^3/kg)	D (m^2/s)
HTO	0	0	3.0×10^{-11}
Br-82	0	0	3.0×10^{-11}
Na-22	7×10^{-7}	1.4×10^{-6}	1.6×10^{-11}
Ca-47	4×10^{-6}	5.2×10^{-6}	1.0×10^{-11}
Sr-85	8×10^{-6}	4.7×10^{-6}	1.0×10^{-11}
Ba-131	2×10^{-4}	2.0×10^{-4}	1.0×10^{-11}
Ba-133	2×10^{-4}	2.0×10^{-4}	1.0×10^{-11}
Rb-86	5×10^{-4}	4.0×10^{-4}	2.5×10^{-11}
Cs-134	8×10^{-3}	6.0×10^{-3}	2.5×10^{-11}

A matrix porosity of $\theta = 0.004$ and $\rho = 2700\ \mathrm{kg/m^3}$ based on Andersson et al. (1997) are used. The values of K_a, K_d^m and D are obtained from the laboratory. K_d^g and α are fitted values for gauge material; the same values of K_d^g and α are used as in the evaluation of Na, Sr and Rb in STT-1.

The resulting (deterministic) travel times (hours) and mass recoveries for pulse input are

Tracer	t_5	t_{50}	t_{95}	*Recovery*
HTO	4.8	12.3	330.1	0.97
Br-82	4.8	12.3	330.1	0.94
Na-22	6.1	20.9	336.5	0.99
Ca-47	7.6	27.2	436.8	0.95
Sr-85	8.6	30.3	414.8	0.99
Ba-131	32.6	164.4	9946.0	0.82
Ba-133	32.6	164.4	9946.0	0.90
Rb-86	88.4	745.2	46646.3	0.61
Cs-134	1318.7	15773.5	861787.5	0.16

The resulting (deterministic) travel times (hours) and mass recoveries for experimental input are

Tracer	t_5	t_{50}	t_{95}	*Recovery*
HTO	8.5	57.4	295.1	0.99
Br-82	8.3	52.4	231.3	0.95
Na-22	11.3	66.2	374.0	1.00
Ca-47	14.6	67.8	348.9	0.96
Sr-85	16.8	79.0	446.8	1.00
Ba-131	57.3	279.2	6389.4	0.83
Ba-133	56.8	283.1	6853.1	0.90
Rb-86	118.4	660.2	8715.7	0.67
Cs-134	1556.8	14304.3	459294.3	0.15

The recovery is calculated at the termination time provided by the Task Force Secretariate.

References

Andersson, P., et al., TRUE 1st stage tracer test programme, Experimental plan for tests with sorbing tracers at the TRUE-1 site, SKB Äspö HRL-97-07, 1997.

Cvetkovic, V., H. Cheng and J.O. Selroos, Evaluation of TRUE-1 sorbing tracer experiments at Äspö: Theory and applications, SKB International Cooperation Report (in preparation).

TRUE Task 4E&F channel network model

L Moreno (KTH-KAT)

TRUE - Task 4E-F
Channel Network Model

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KTH

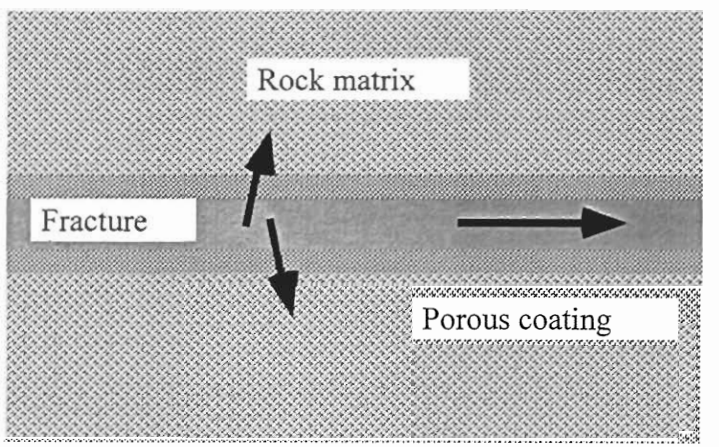
Outline

- Solute transport in fractured media
- Tracer tests with sorbing tracers
- Discussion of prediction results
- Uncertainties

KTH

Solute transport in fractured media

- By advection in the fracture/channels
- Sorption onto fracture surface /filling
- Diffusion/sorption in the rock matrix.
- Diffusion into stagnant water



KTH

Solute transport

- **Key entities**
  - **Flow-wetted surface / flow rate**
  - **Flow porosity**
  - **Diffusion and sorption properties**

$$\frac{C}{C_o} = erfc\left[\frac{\left(D_e K_d \rho_p\right)^{0.5}}{\left(t - t_a\right)^{0.5}} \frac{L \cdot W}{Q}\right]$$

KTH

Prediction results

- **Sorbing tracer tests. No good prediction**
  - **Predicted breakthrough times were shorter**
  - **To match results, we required (Cs)**
    - » **900 times larger $D_e K_d \rho_p$**
    - » **30 times larger Flow-wetted surface**
    - » **30 smaller water flow rate**

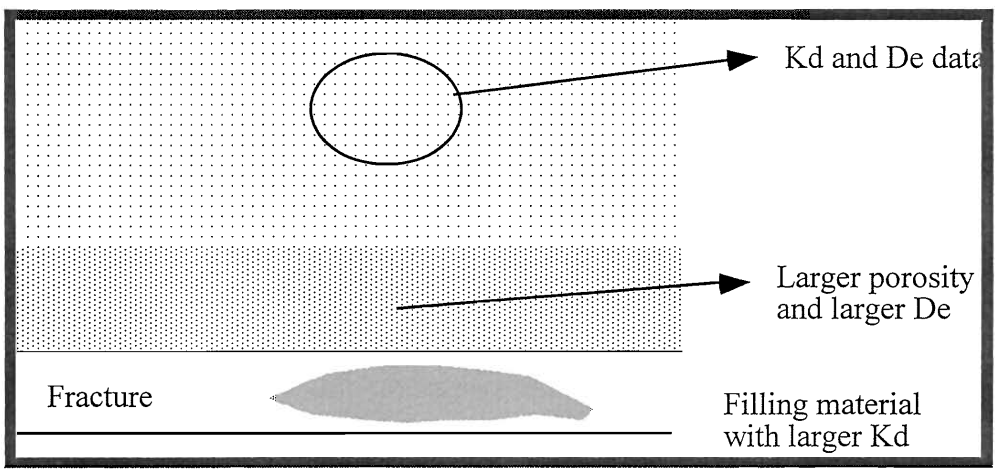
KTH

Discussion

- **The long breakthrough times could be explained by:**
  - **Larger diffusion/sorption**
  - **Sorption on gouge / filling**
  - **Flow rate smaller than the average**
  - **Diffusion into stagnant water**

KTH

Larger diffusion/sorption



VETENSKAP OCH KONST

KTH

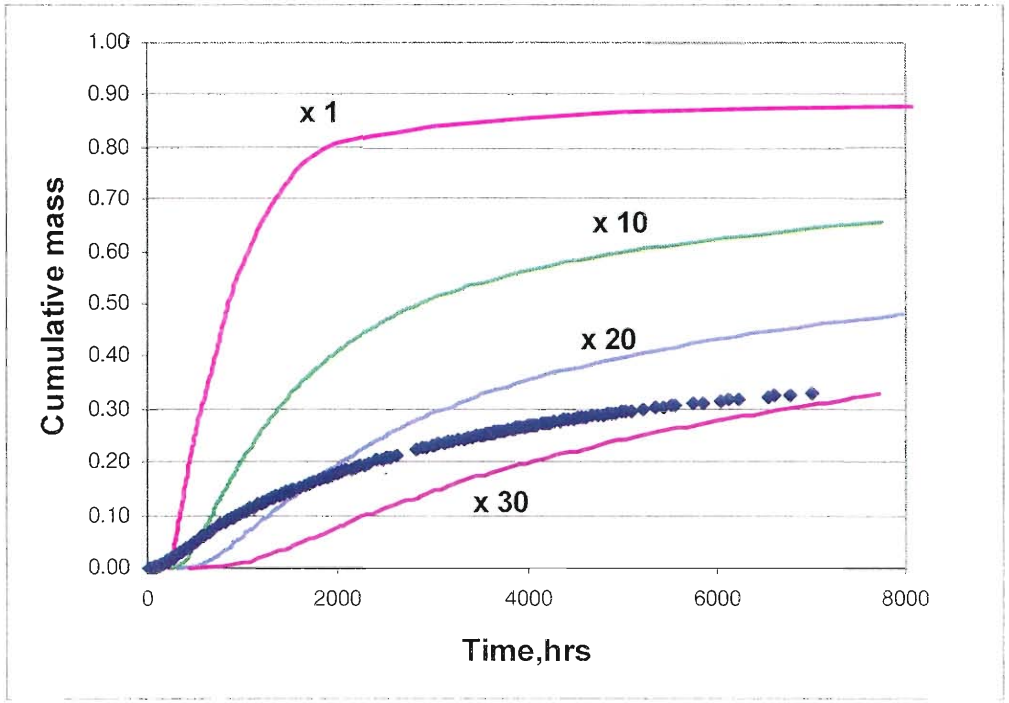
Larger diffusion/sorption

- **Diffusion data near the fracture**

Thickness of layer	Porosity	Pore diffusivity $D_p, m^2/s$	Effective diffusivity $D_e, m^2/s$
Gouge, 1 mm	-	Infinity	Infinity
Alt. rock, 1 mm	0.05	$2 \cdot 10^{-10}$	$1 \cdot 10^{-11}$
Alt. rock, 5 mm	0.015	$1 \cdot 10^{-10}$	$1.5 \cdot 10^{-12}$
Alt. rock, 25 mm	0.015	$1 \cdot 10^{-10}$	$1.5 \cdot 10^{-12}$
Virgin rock	0.004	$0.5 \cdot 10^{-10}$	$2 \cdot 10^{-13}$

KTH

Larger diffusion/sorption



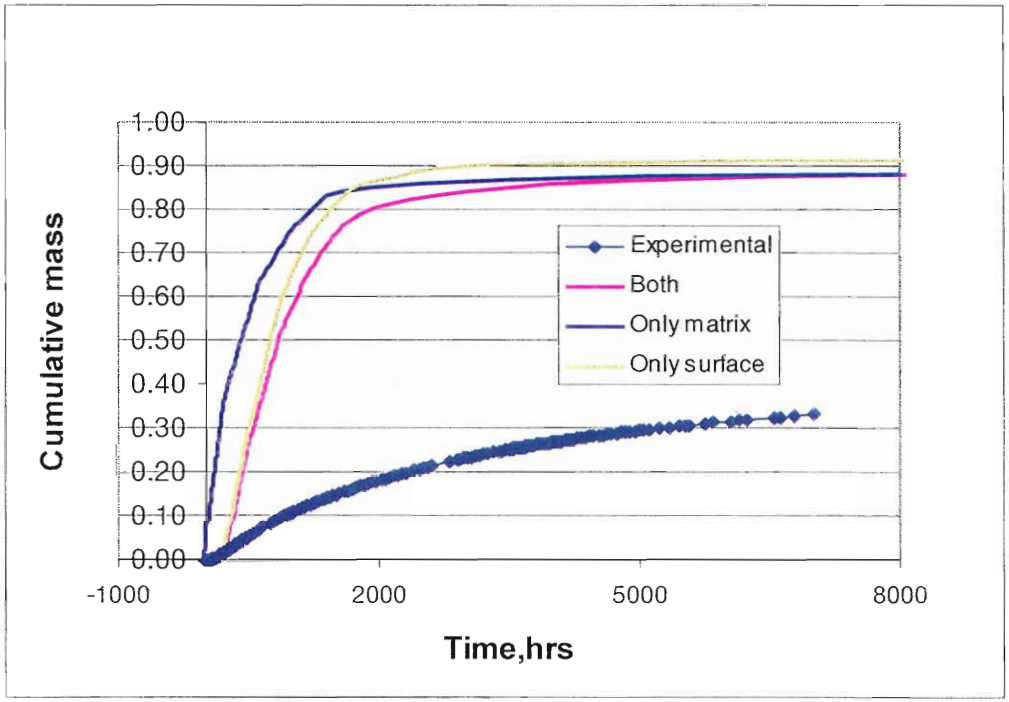
KTH

Larger diffusion/sorption

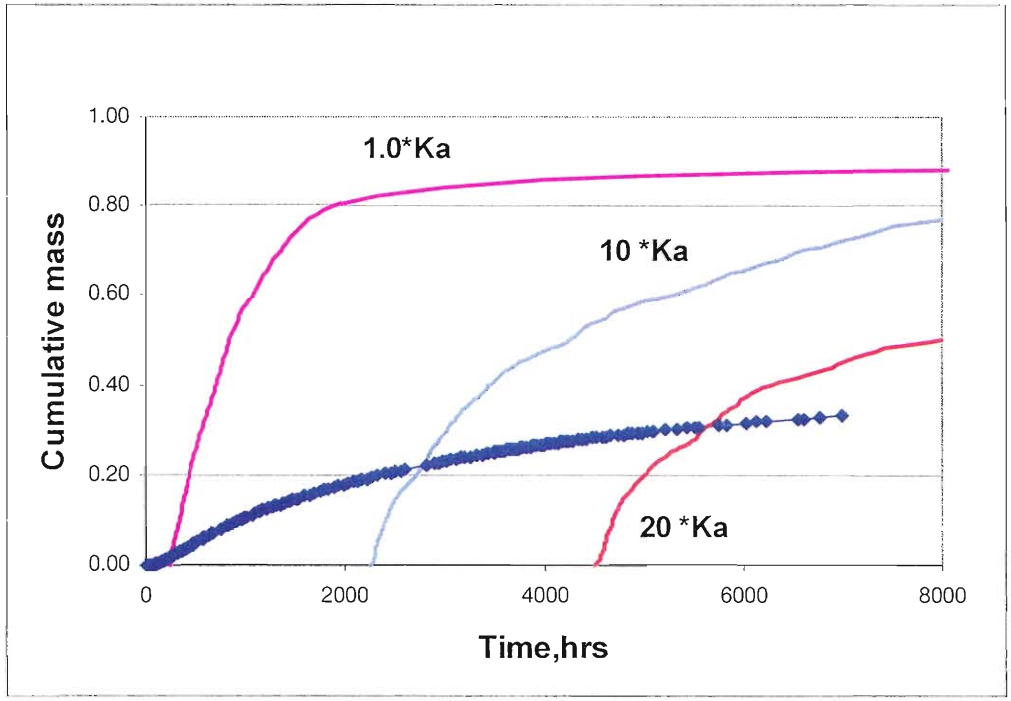
- **900 times larger diffusion or/and sorption is required**
- **It can partially explain the results**

KTH

Sorption onto the fracture surface / filling



Sorption onto the fracture surface / filling



Sorption onto the fracture surface / filling

- Surface sorption (instantaneous) can not explain the results
- Kinetics effects are required
  - Gouge (diffusion)
  - Sorption kinetics

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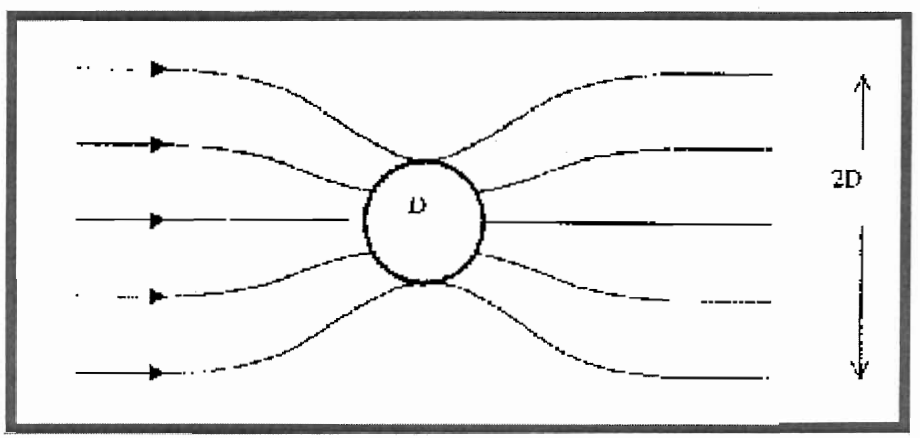
Injection located at zone with lower water flow rate

- Fracture aperture
  - Residence time ~ 10hrs
  - Fracture aperture = 3 mm
- If there is filling in the fracture a larger aperture is required

Injection located at zone with lower water flow rate

- **Flow through injection section**
  - **Flow equivalent to two-diameter**



Injection located at zone with lower water flow rate

- **Drawdown**

Borehole	KXTT1	KXTT2	KXTT3	KXTT4	KA3005
Transmissivity m2/s	8.3E-9	5.9E-9	2.1E-7	1.8E-8	2.7E-8
Drawdown	0.62	2.23	3.12	0.32	0.28
Recoverey	high	zero	Extract	high	zero

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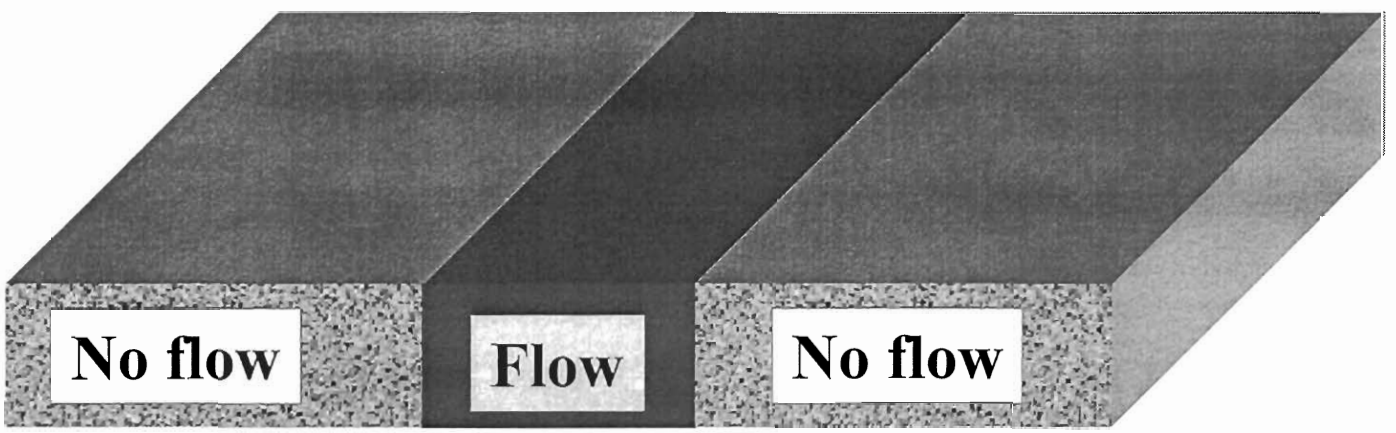
Injection located at zone with lower water flow rate

- A smaller flow can partially explain the longer residence times for the non-sorbing tracer
- A water flow rate 30 times smaller is required

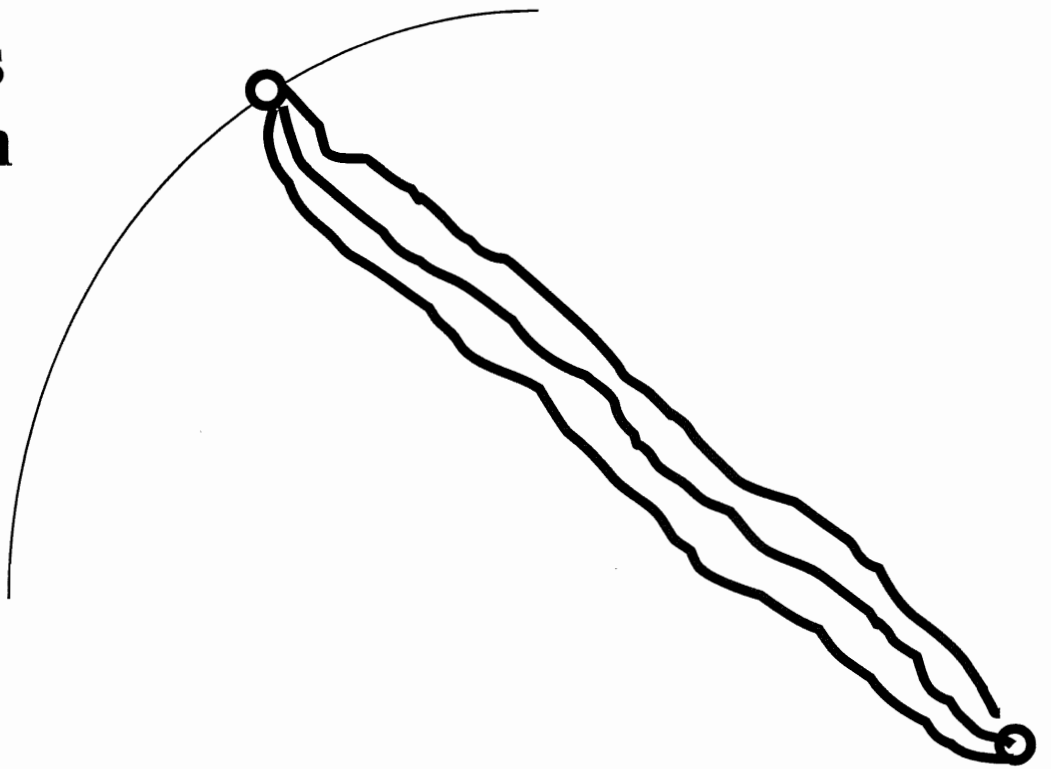
Diffusion in stagnant water in the fracture

- **Increases retardation effect. Important for large fracture apertures**



Diffusion in stagnant water in the fracture

- Several Channels increase diffusion into stagnant water
- Sorbing species require several channels to match experiments



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Uncertainties

- **Data varying in a wide interval**
  - **Sorption and diffusion**
    - » **Rock type, particle size, alteration**
- **Varying flow around the extraction hole. Channels**
- **Anomalous head field**

Results from RC-4 tracer experiment

P Andersson (Geosigma)

RESULTS FROM THE RC-4 TRACER EXPERIMENT

Presentation at the 13th Meeting of the Task Force on Modelling of Groundwater Flow and Transport of Solutes

Carlsbad, New Mexico
February 8-11, 2000

Peter Andersson
GEOSIGMA AB

RC-4 CONSERVATIVE TRACER TESTS

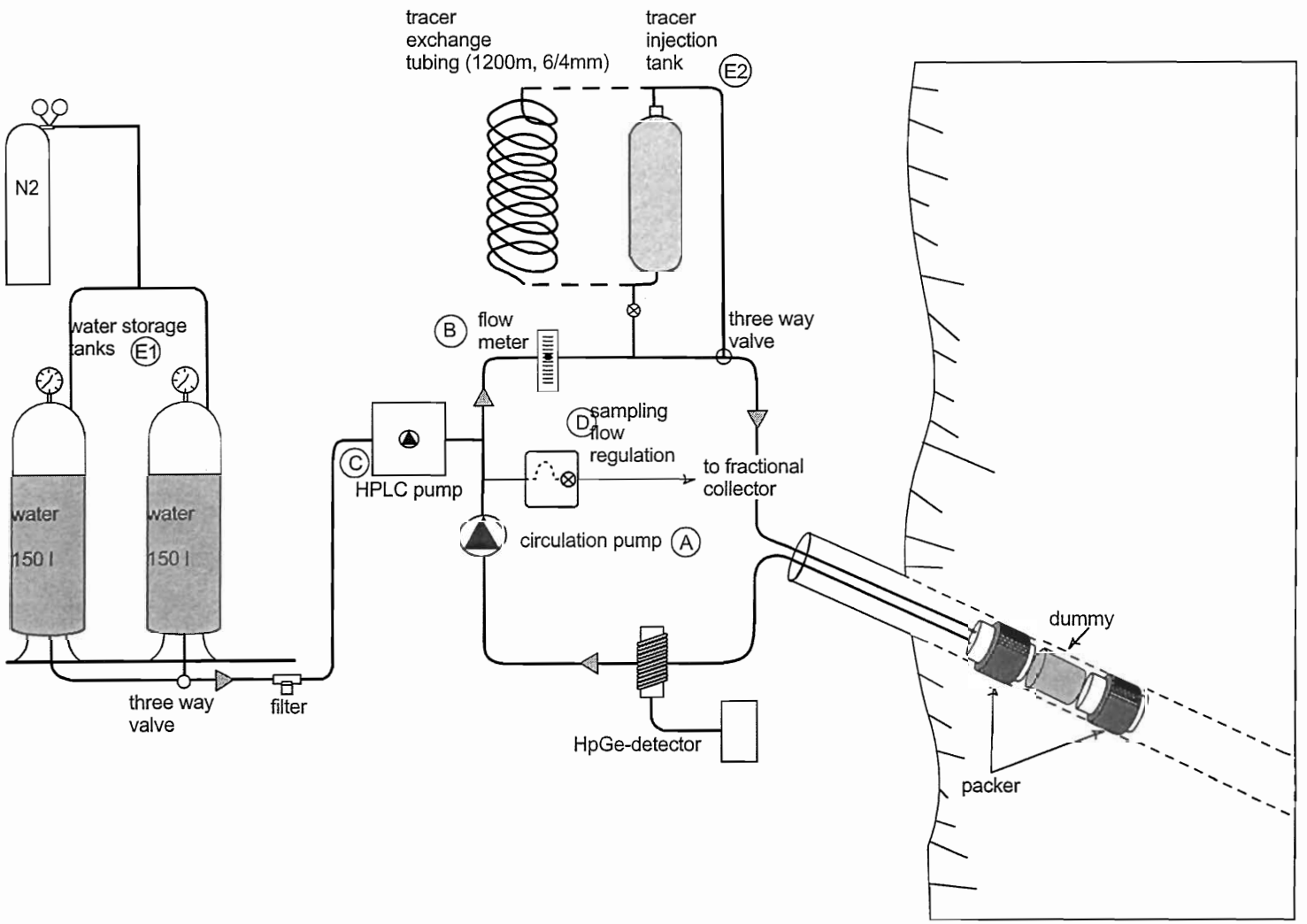
- **OBJECTIVES:**

- To test a new down-hole equipment in-situ under ambient flow and pressure conditions

- To demonstrate that a well-defined tracer pulse injection can be performed

- To characterise a new flow path in Feature A

TRUE-1 CONSERVATIVE TRACER TESTS

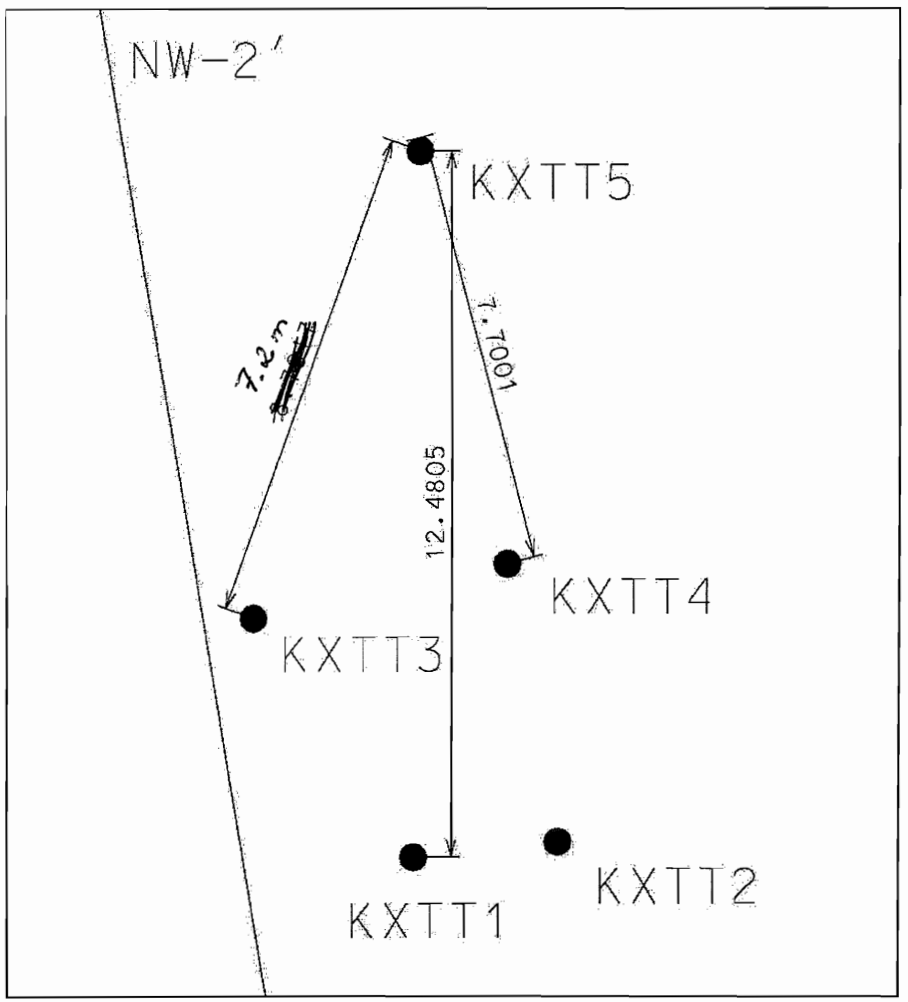


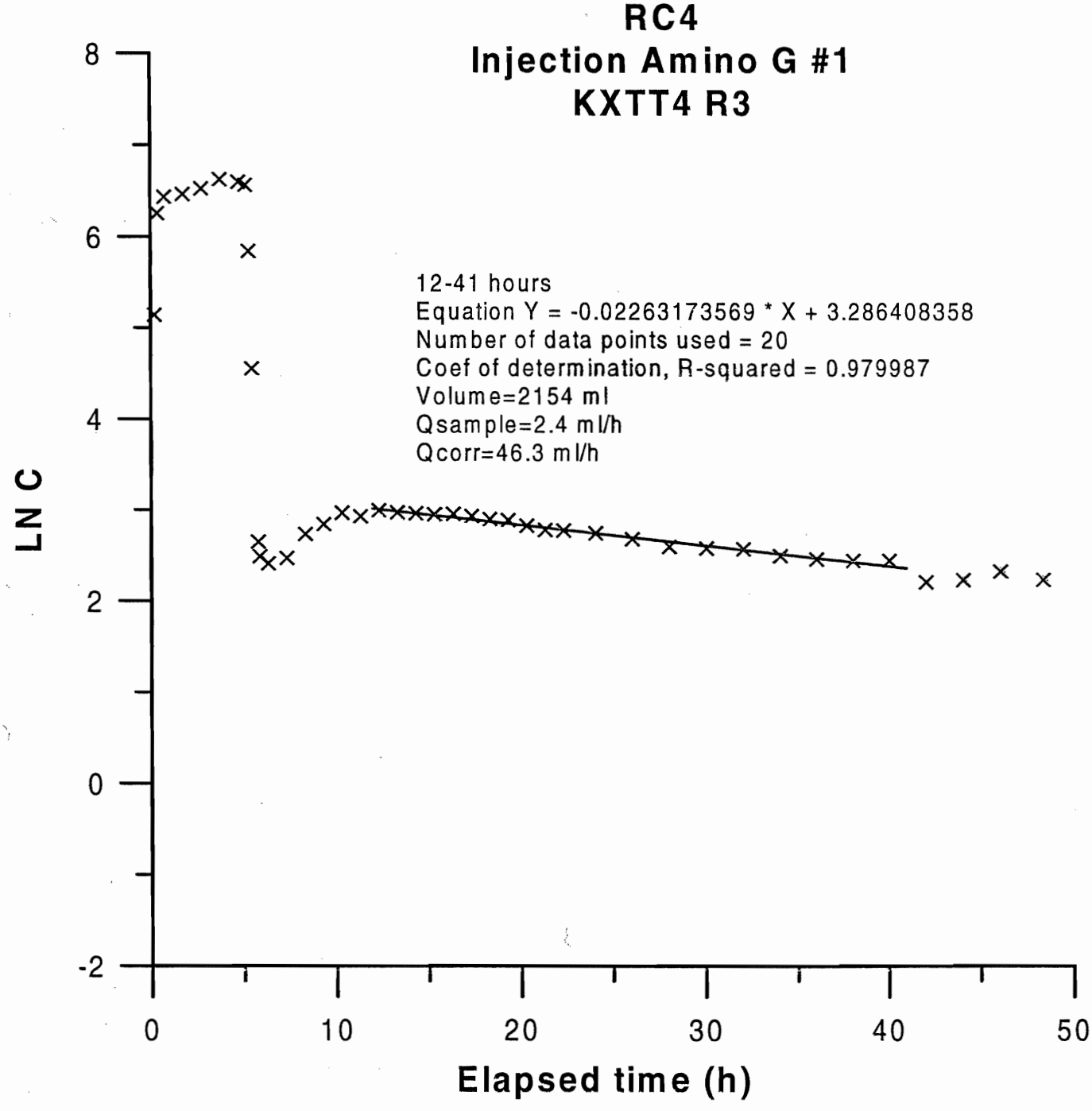
RC-4 CONSERVATIVE TRACER TESTS

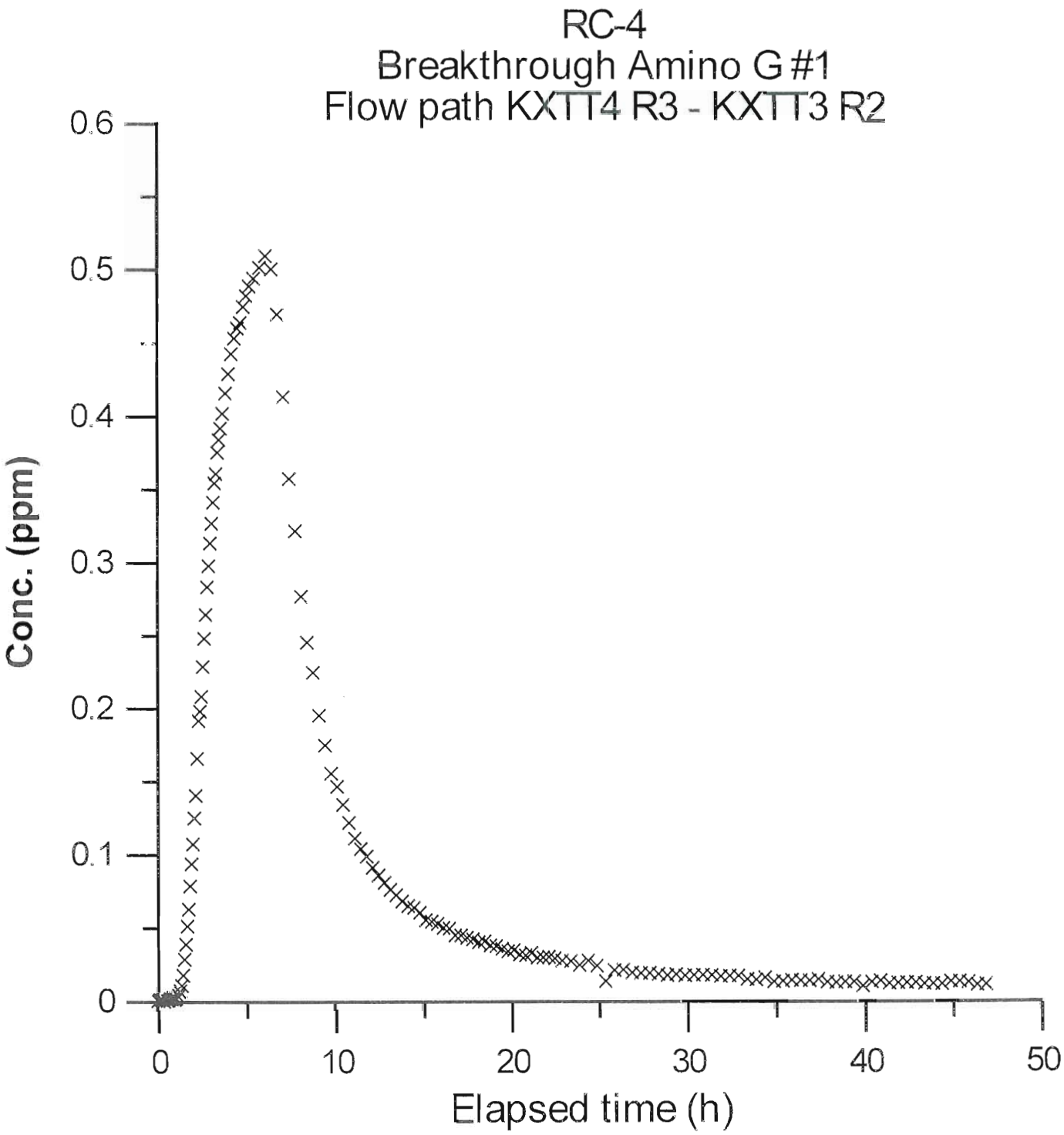
IMPROVEMENT OF EQUIPMENT

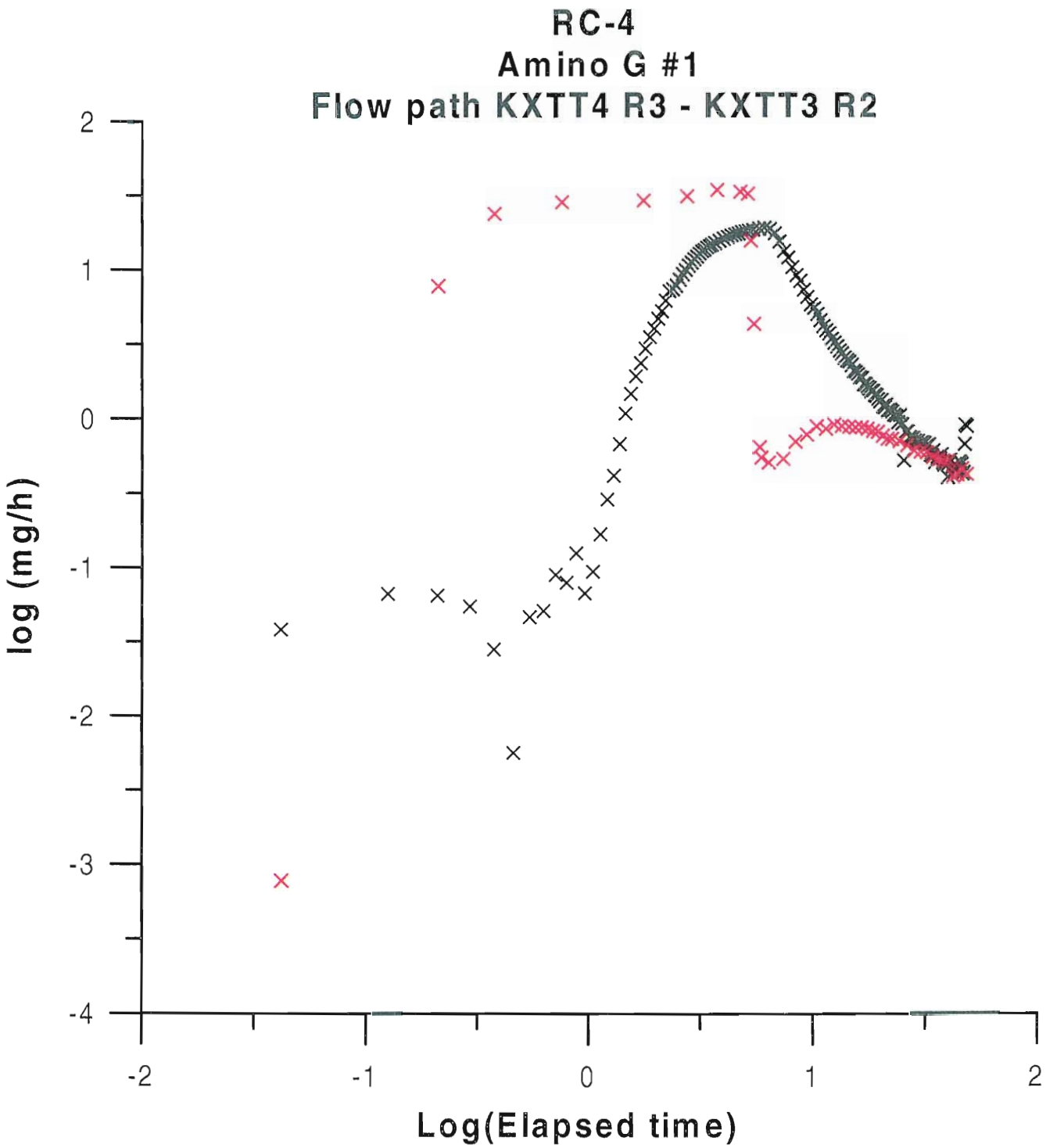
- Minimisation of volume, 90% reduction
- No stagnant volumes

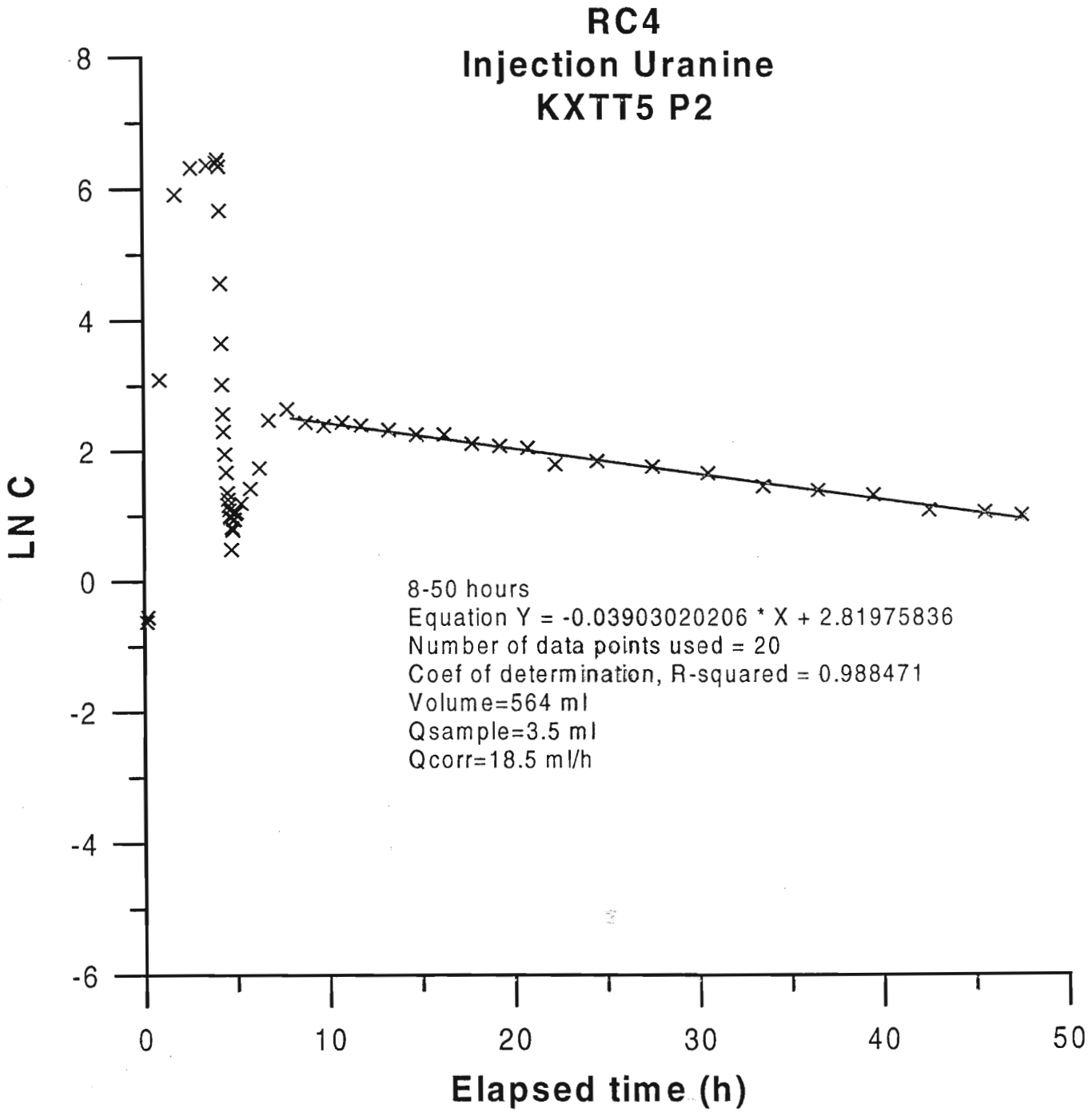
RC-4 GEOMETRY

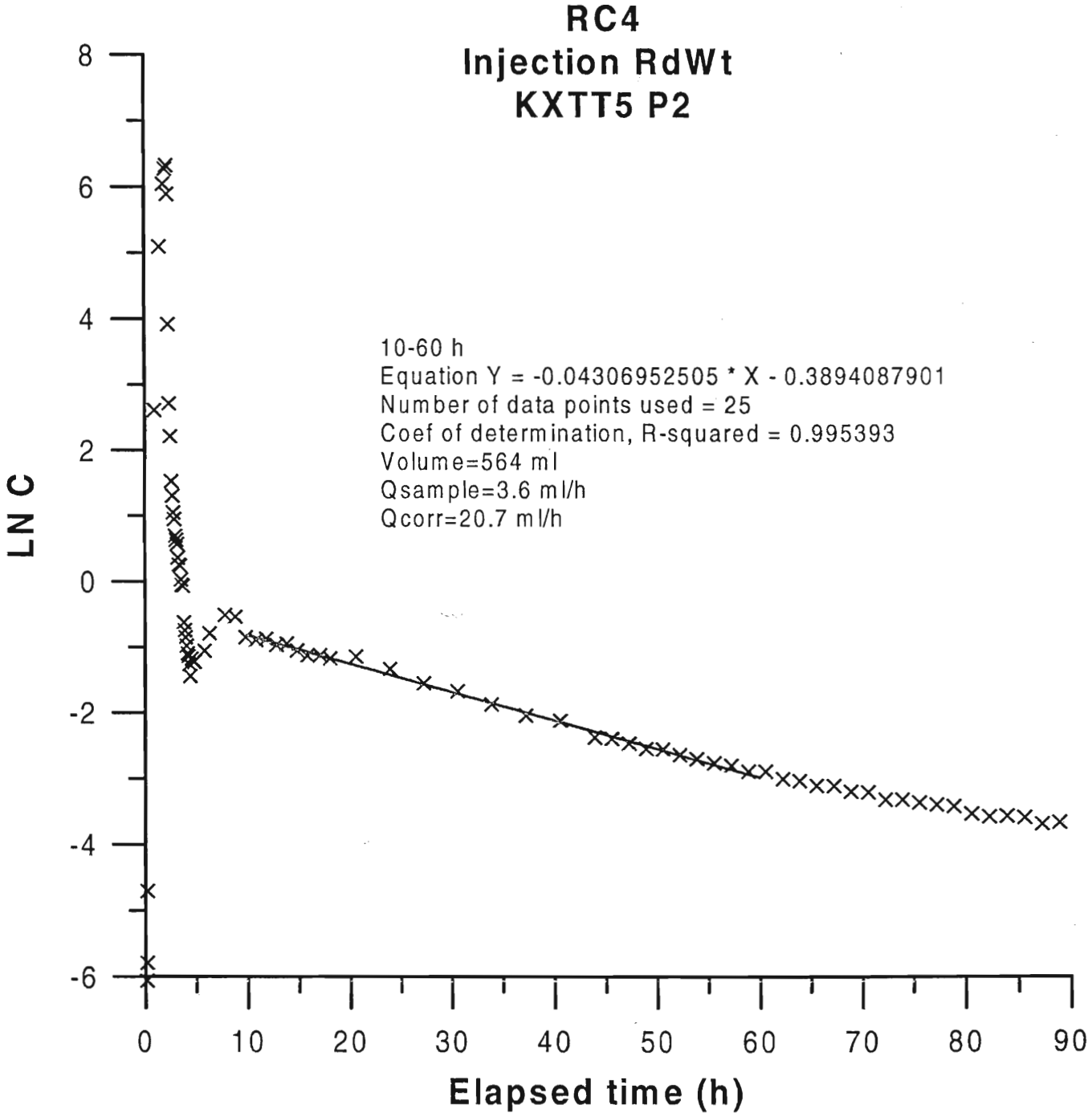


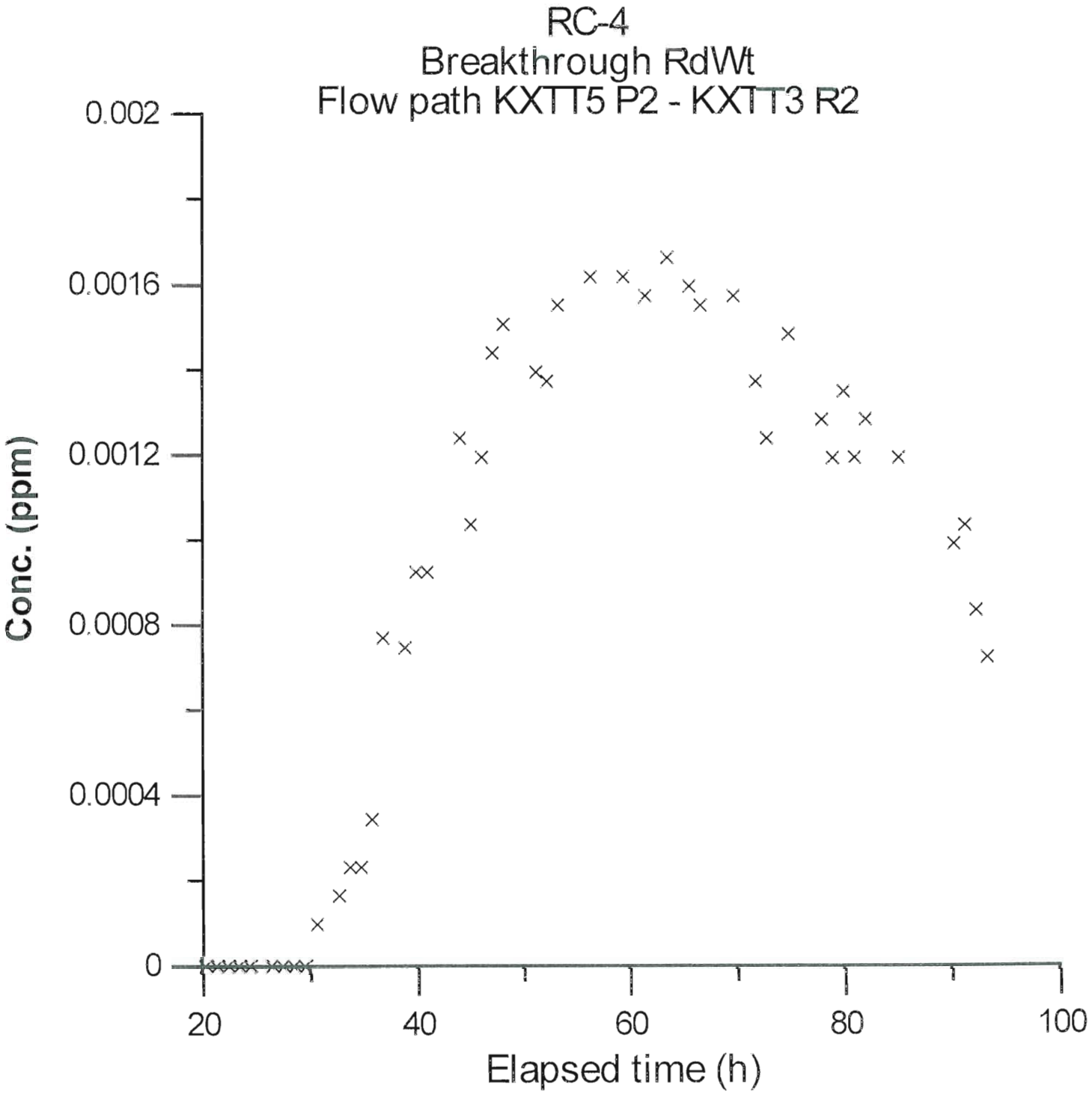

RC4
Injection Amino G #1
KXTT4 R3
12-41 hours
Equation Y = -0.02263173569 * X + 3.286408358
Number of data points used = 20
Coef of determination, R-squared = 0.979987
Volume=2154 ml
Qsample=2.4 ml/h
Qcorr=46.3 ml/h
LN C
8
6
4
2
0
-2
0
10
20
30
40
50
Elapsed time (h)

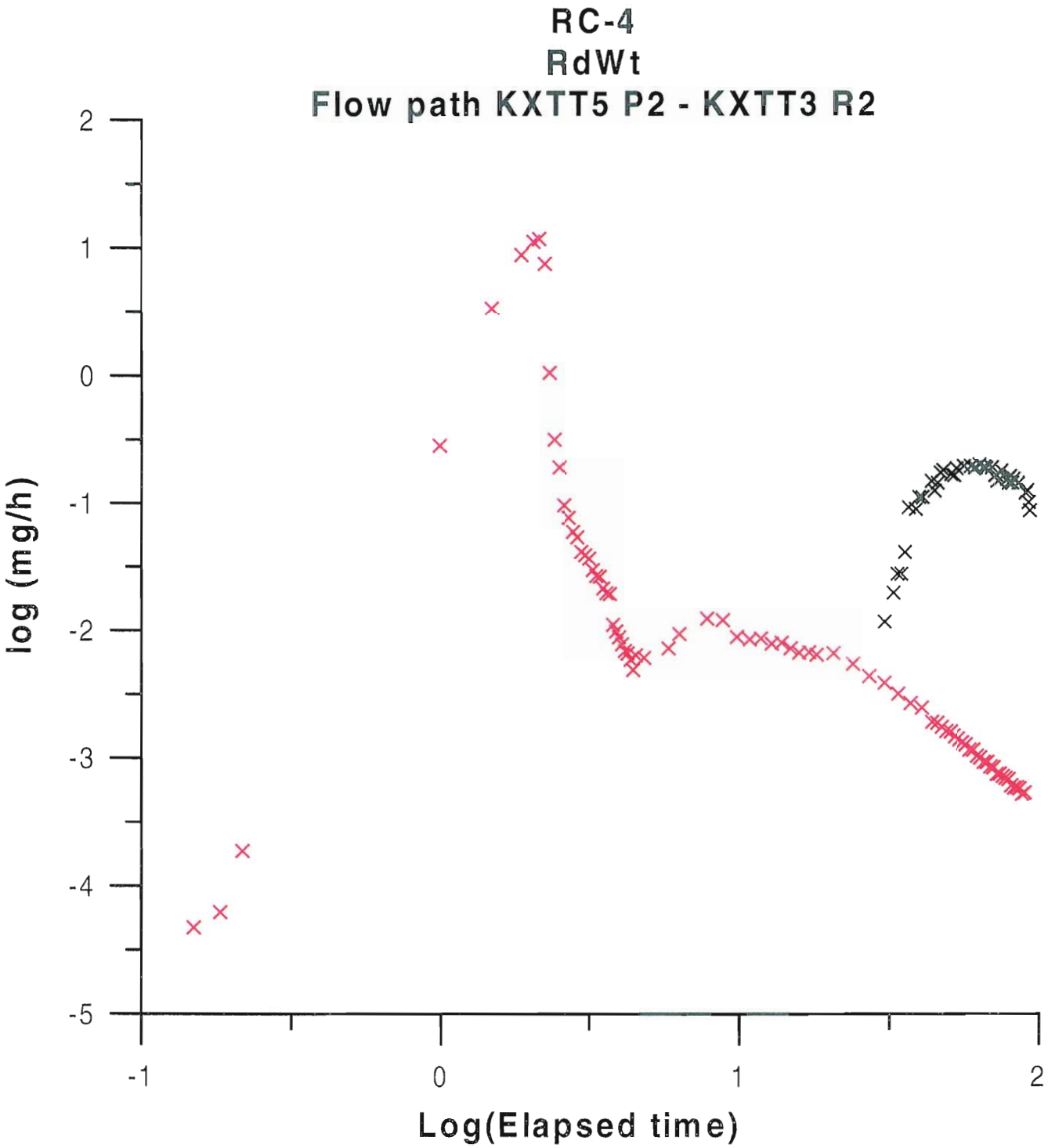

RC-4
Breakthrough Amino G #1
Flow path KXTT4 R3 - KXTT3 R2
Conc. (ppm)
0.6
0.5
0.4
0.3
0.2
0.1
0
0
10
20
30
40
50
Elapsed time (h)

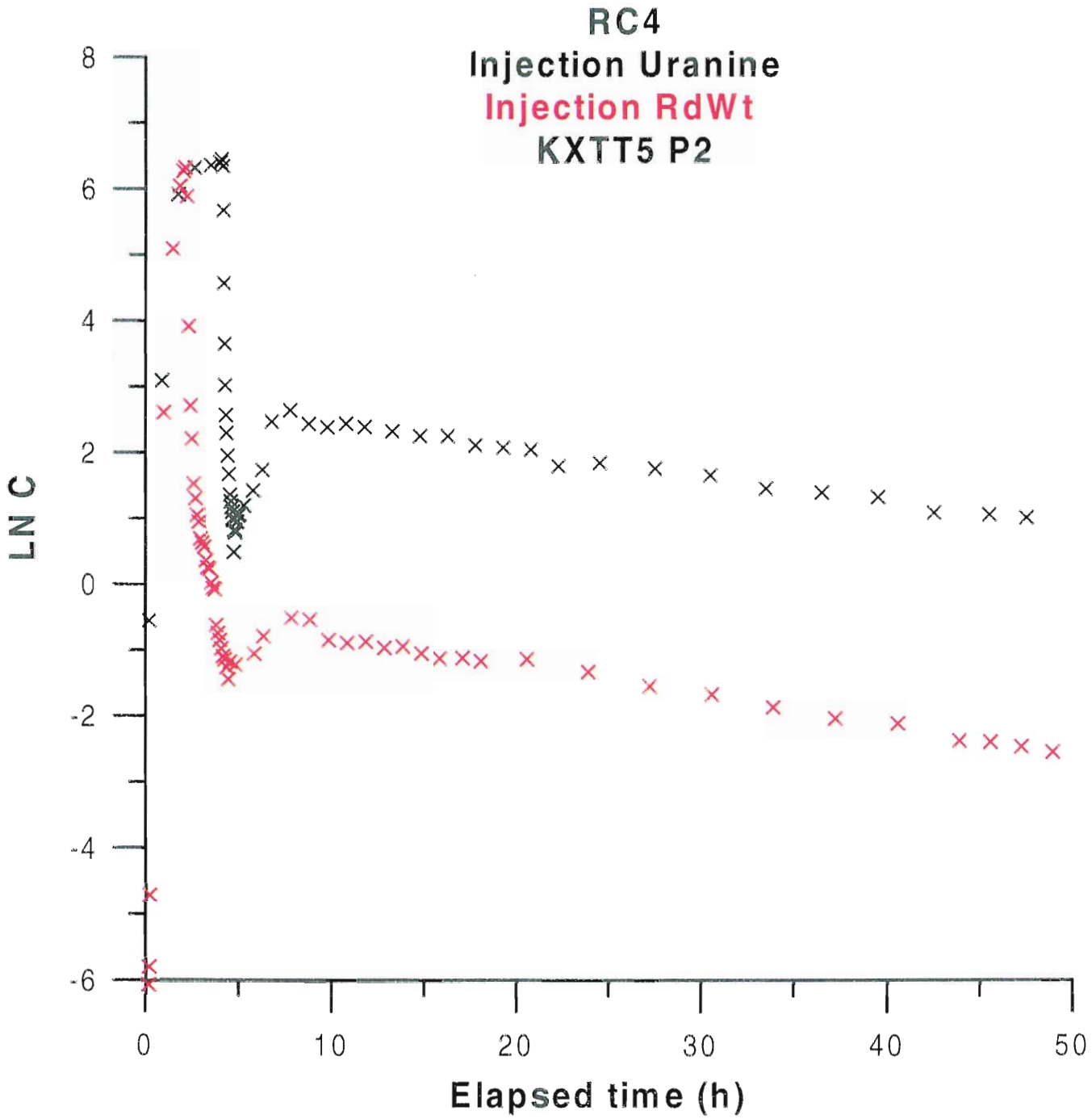

RC-4
Amino G #1
Flow path KXTT4 R3 - KXTT3 R2
log (mg/h)
2
1
0
-1
-2
-3
-4
-2
-1
0
1
2
Log(Elapsed time)

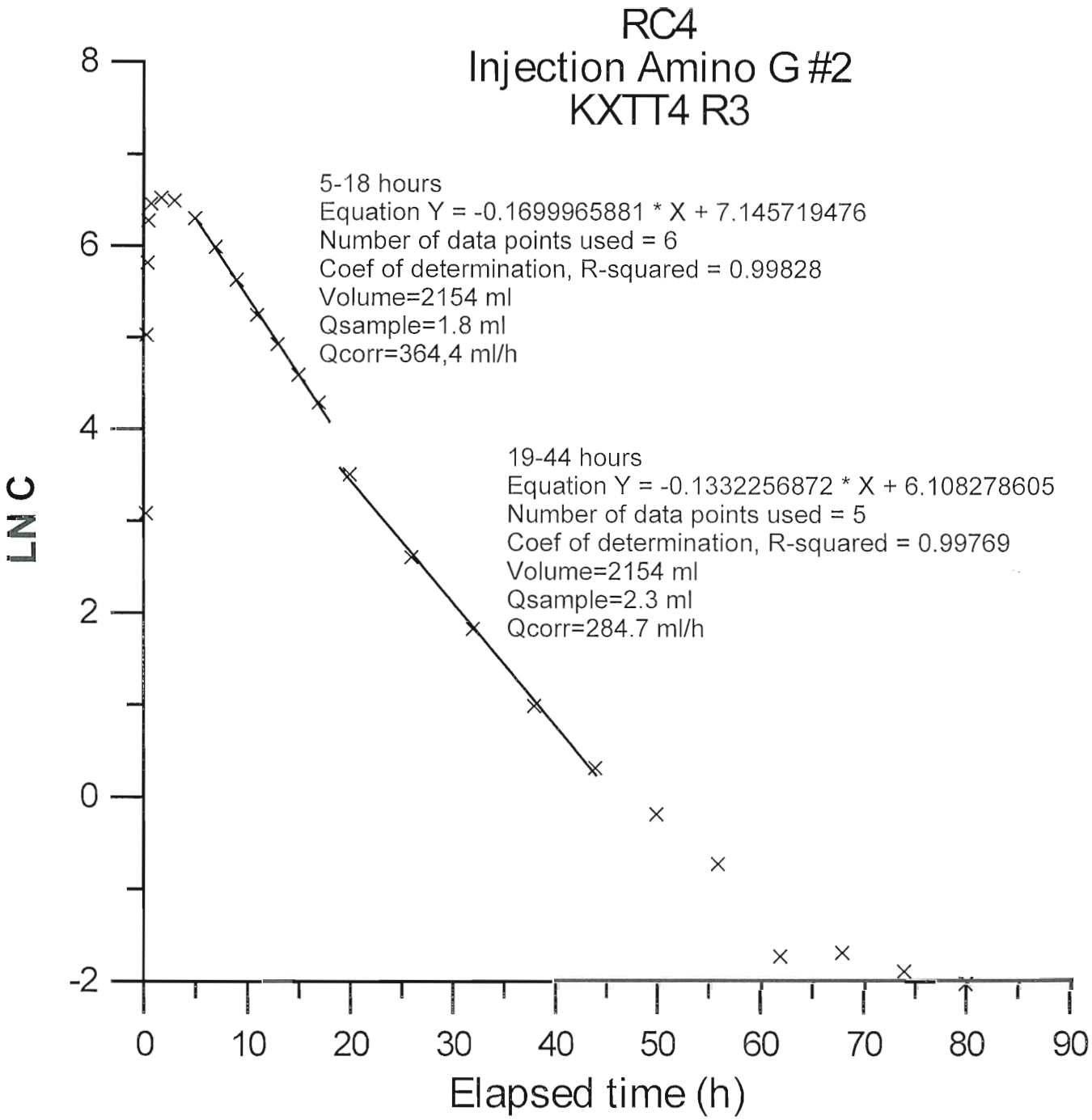

RC4
Injection Uranine
KXTT5 P2
LN C
8
6
4
2
0
-2
-4
-6
0
10
20
30
40
50
Elapsed time (h)
8-50 hours
Equation Y = -0.03903020206 * X + 2.81975836
Number of data points used = 20
Coef of determination, R-squared = 0.988471
Volume=564 ml
Qsample=3.5 ml
Qcorr=18.5 ml/h

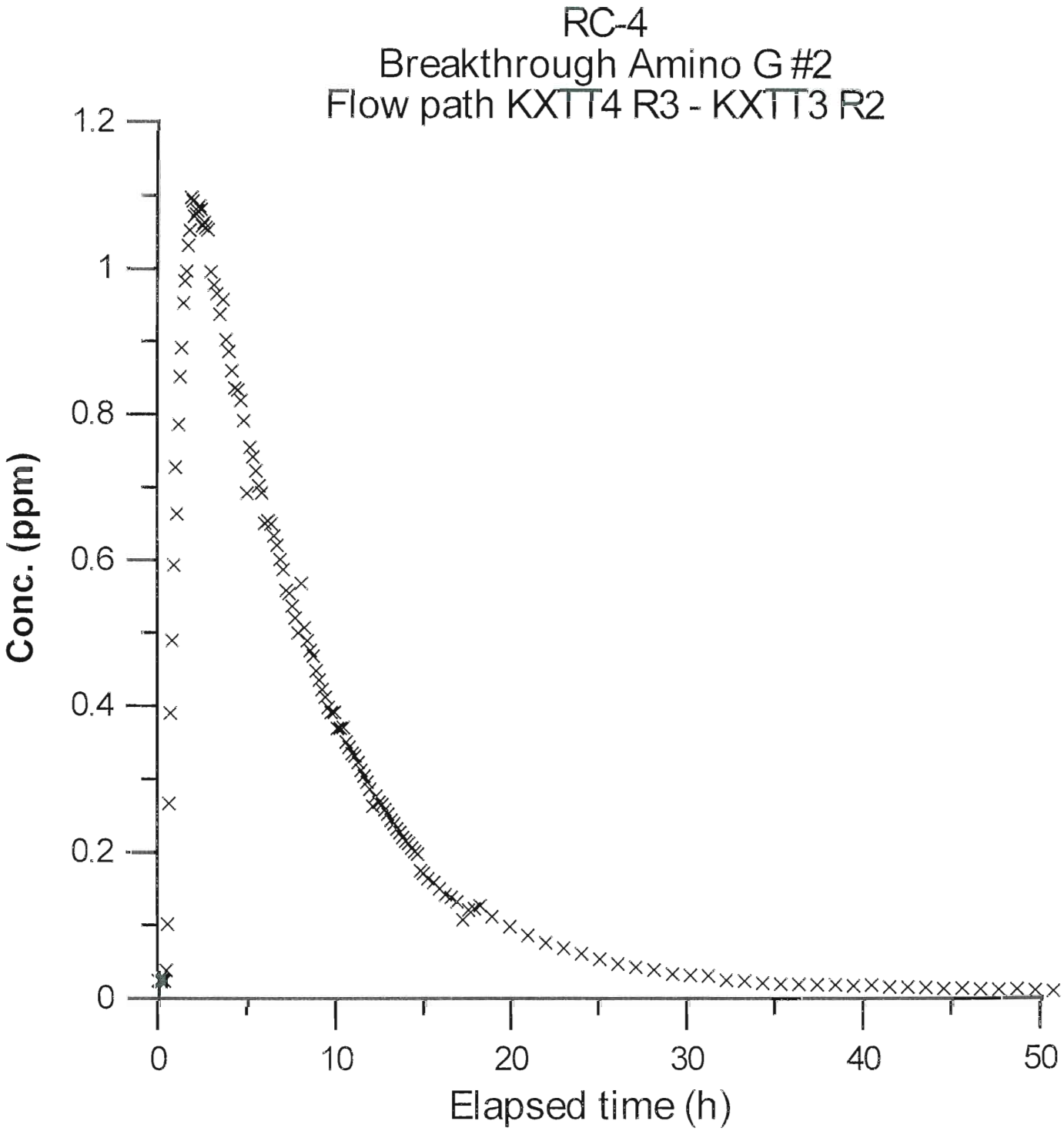

RC4
Injection RdWt
KXTT5 P2
10-60 h
Equation Y = -0.04306952505 * X - 0.3894087901
Number of data points used = 25
Coef of determination, R-squared = 0.995393
Volume=564 ml
Qsample=3.6 ml/h
Qcorr=20.7 ml/h
LN C
8
6
4
2
0
-2
-4
-6
0
10
20
30
40
50
60
70
80
90
Elapsed time (h)

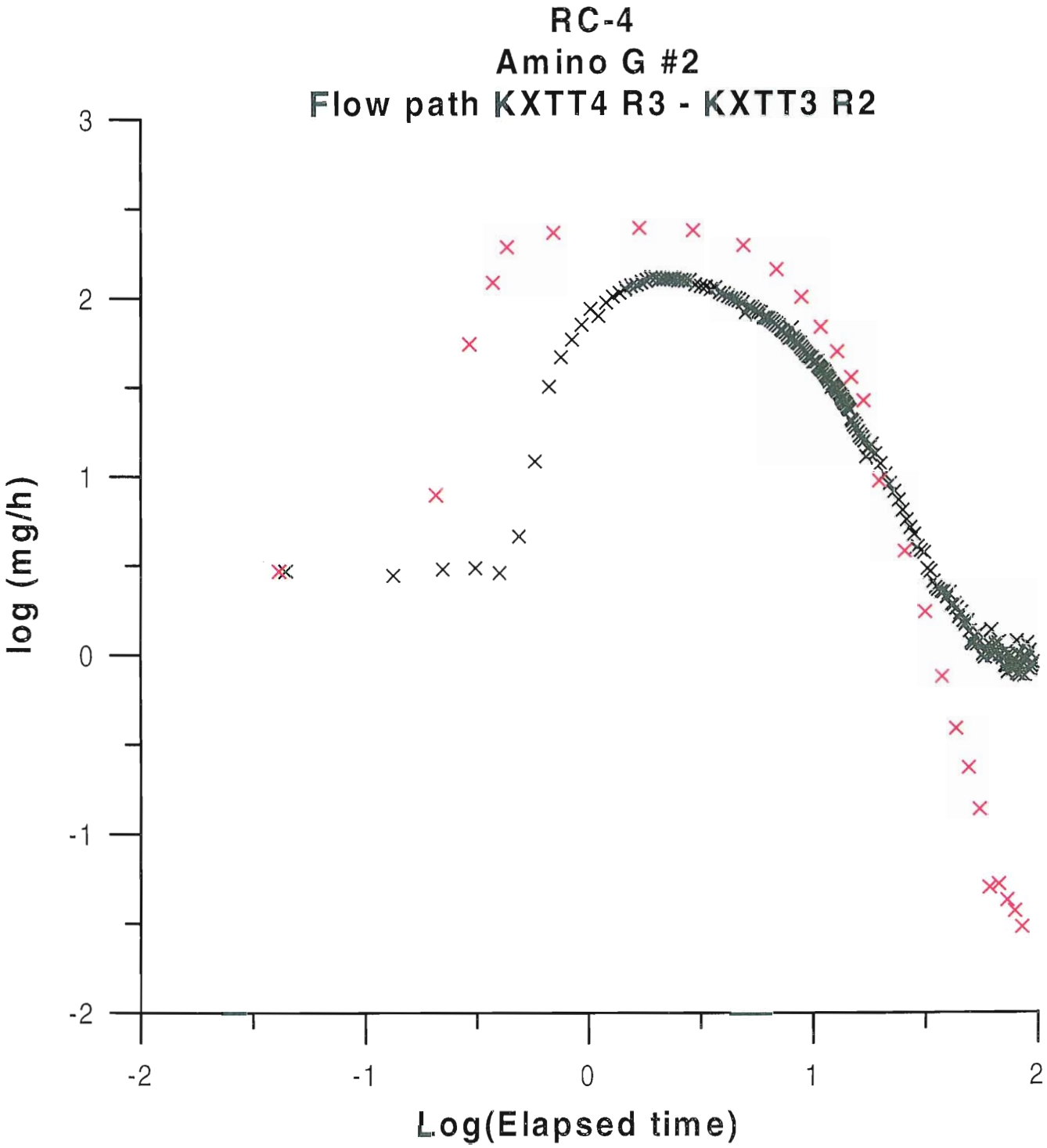

RC-4
Breakthrough RdWt
Flow path KXTT5 P2 - KXTT3 R2
0.002
0.0016
0.0012
0.0008
0.0004
0
Conc. (ppm)
20
40
60
80
100
Elapsed time (h)


RC-4
RdWt
Flow path KXTT5 P2 - KXTT3 R2
log (mg/h)
2
1
0
-1
-2
-3
-4
-5
-1
0
1
2
Log(Elapsed time)


RC4
Injection Uranine
Injection RdWt
KXTT5 P2
LN C
8
6
4
2
0
-2
-4
-6
0
10
20
30
40
50
Elapsed time (h)


RC4
Injection Amino G #2
KXTT4 R3
5-18 hours
Equation Y = -0.1699965881 * X + 7.145719476
Number of data points used = 6
Coef of determination, R-squared = 0.99828
Volume=2154 ml
Qsample=1.8 ml
Qcorr=364,4 ml/h
19-44 hours
Equation Y = -0.1332256872 * X + 6.108278605
Number of data points used = 5
Coef of determination, R-squared = 0.99769
Volume=2154 ml
Qsample=2.3 ml
Qcorr=284.7 ml/h
LN C
8
6
4
2
0
-2
0
10
20
30
40
50
60
70
80
90
Elapsed time (h)


RC-4
Breakthrough Amino G #2
Flow path KXTT4 R3 - KXTT3 R2
Conc. (ppm)
1.2
1
0.8
0.6
0.4
0.2
0
0
10
20
30
40
50
Elapsed time (h)


RC-4
Amino G #2
Flow path KXTT4 R3 - KXTT3 R2
log (mg/h)
3
2
1
0
-1
-2
-2
-1
0
1
2
Log(Elapsed time)

RC-4 tracer injections during pumping in KXTT3 R2 (Inj #1 and #2, Q=0.8 l/min, Inj #3 and #4, Q=2.0 l/min)

Inj #	Section	Tracer	Max Conc (ppm)	Inj rate (ml/h)	Exchange efficiency (%)
1	KXTT4 R3	Amino-G Acid	750	46	97
2	KXTT5 P2	Uranine	630	18	98
3	KXTT4 R3	Amino G Acid	700	300	No exchange
4	KXTT5 P2	Rhodamine WT	700	21	99.9

RC-4 tracer test

CONCLUSIONS

- The new borehole equipment in combination with a longer exchange period has significantly improved the tracer pulse injection procedure
- A new flow path , KXTT5 P2 - KXTT3 R2 has been tested in Feature A and found to be connected but more difficult to control
- Additional transport data for the flow path KXTT4 R3 - KXTT3 R2 has been produced for two new strengths of the sink

Results of complementary laboratory experiment

J Byegård and H Johansson (CTH)

nuclear chemistry

NEW LABORATORY EXPERIMENTAL RESULTS FROM THE STUDY OF THE POROSITY, DIFFUSIVITY AND SORPTIVITY OF THE RIM ZONE OF THE FEATURE A

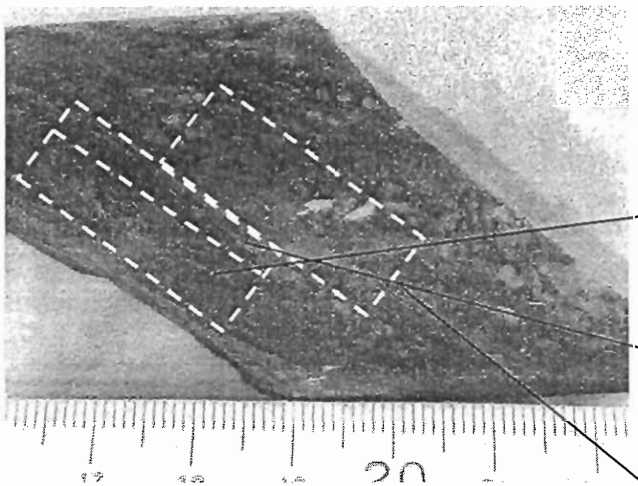
ÄSPÖ TASK FORCE MEETING
8-11 FEBRUARY 2000

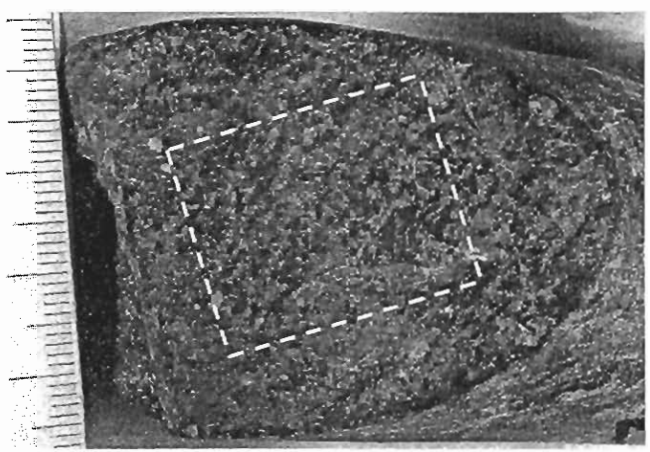
J. BYEGÅRD, H. JOHANSSON
Dep. of Nuclear Chemistry
Chalmers University of Technology

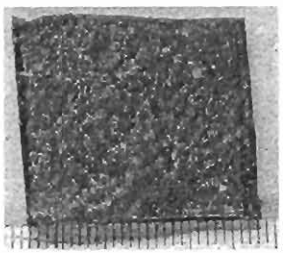
Content

- Detailed porosity and diffusivity measurements of Feature A mylonite and altered diorite
- Penetration profile studies of the KXTT1 sample, exposed to through diffusion experiment for 3 years
- Porosity homogeneity and distribution studies using the ^{14}C-labelled MMA impregnation

Sampling of KXTT2-core

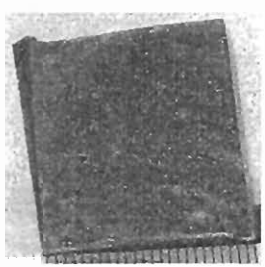






T2A,
outer mylonite,
~5 mm thick

T2B,
inner mylonite,
~3 mm thick

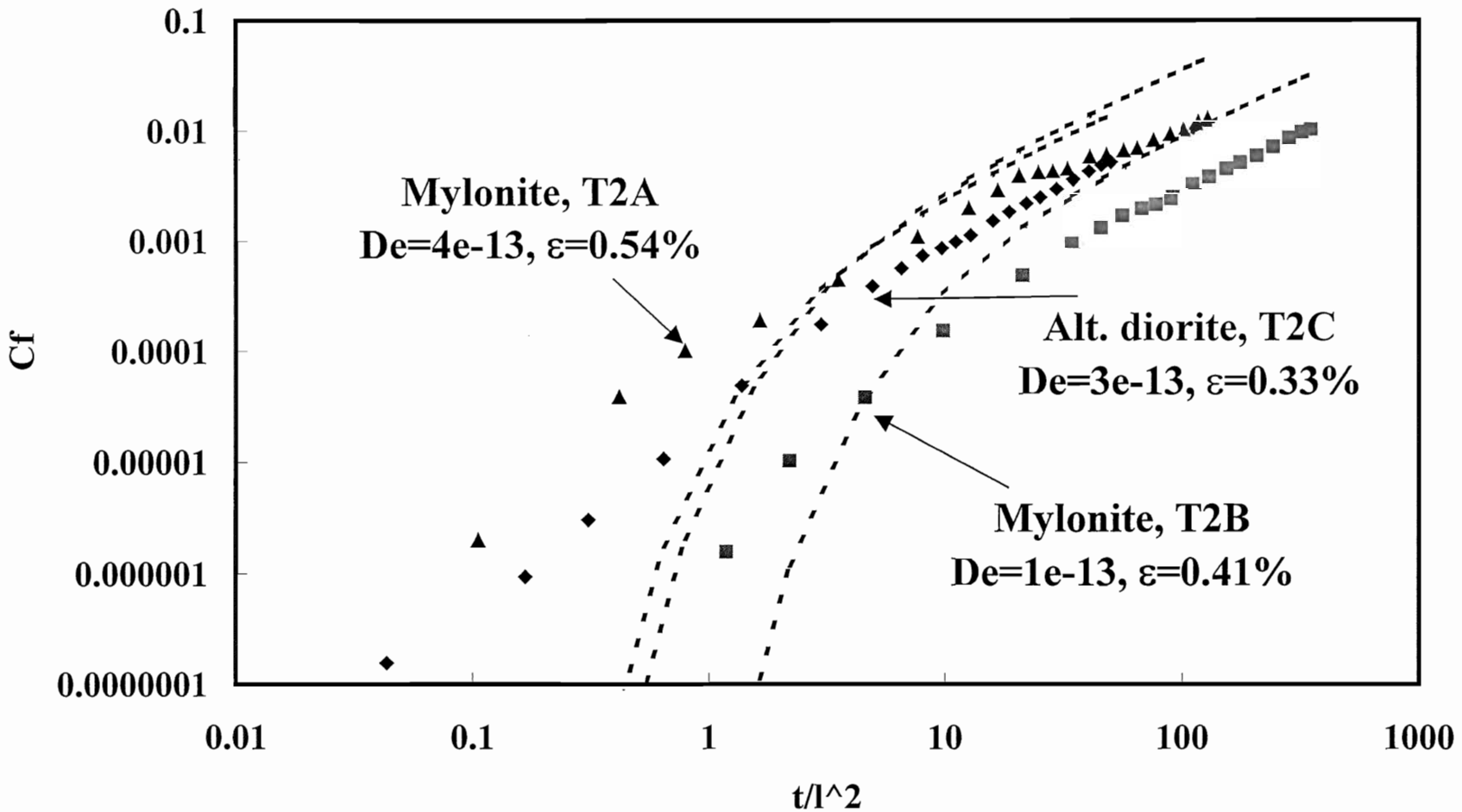


T2C,
Alt. Äspö diorite,
~8 mm thick

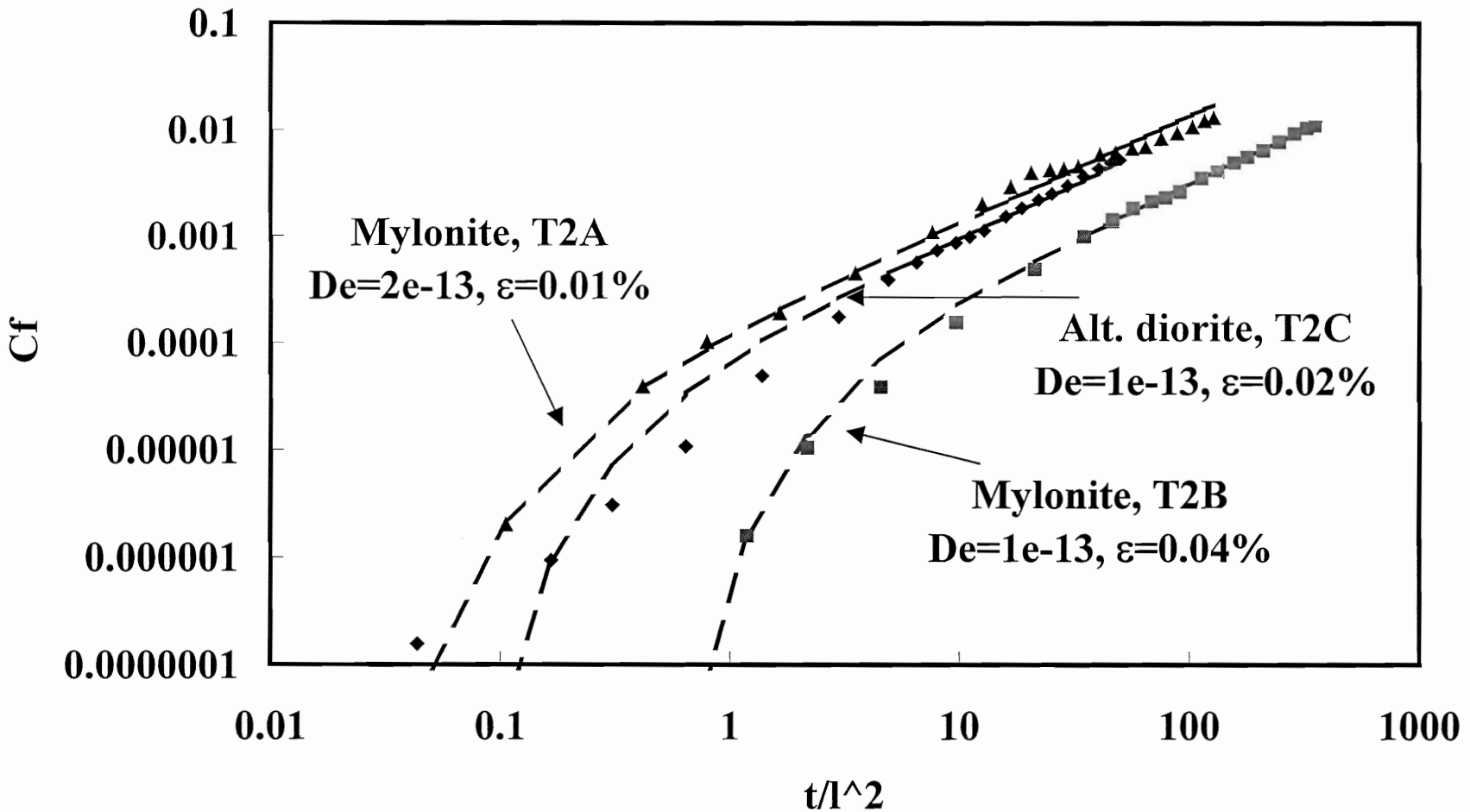
Water Saturation Porosity

Sample	Description	Porosity (vol%)
T2A	Outer mylonite, Feature A surface	0.54
T2B	Inner Mylonite	0.41
T2C	Altered Äspö-diorite	0.33
T2H	Mylonite, "Neighbour" to T2A and T2B, Feature A surface	0.97
	Whole core, before any sawing	0.46

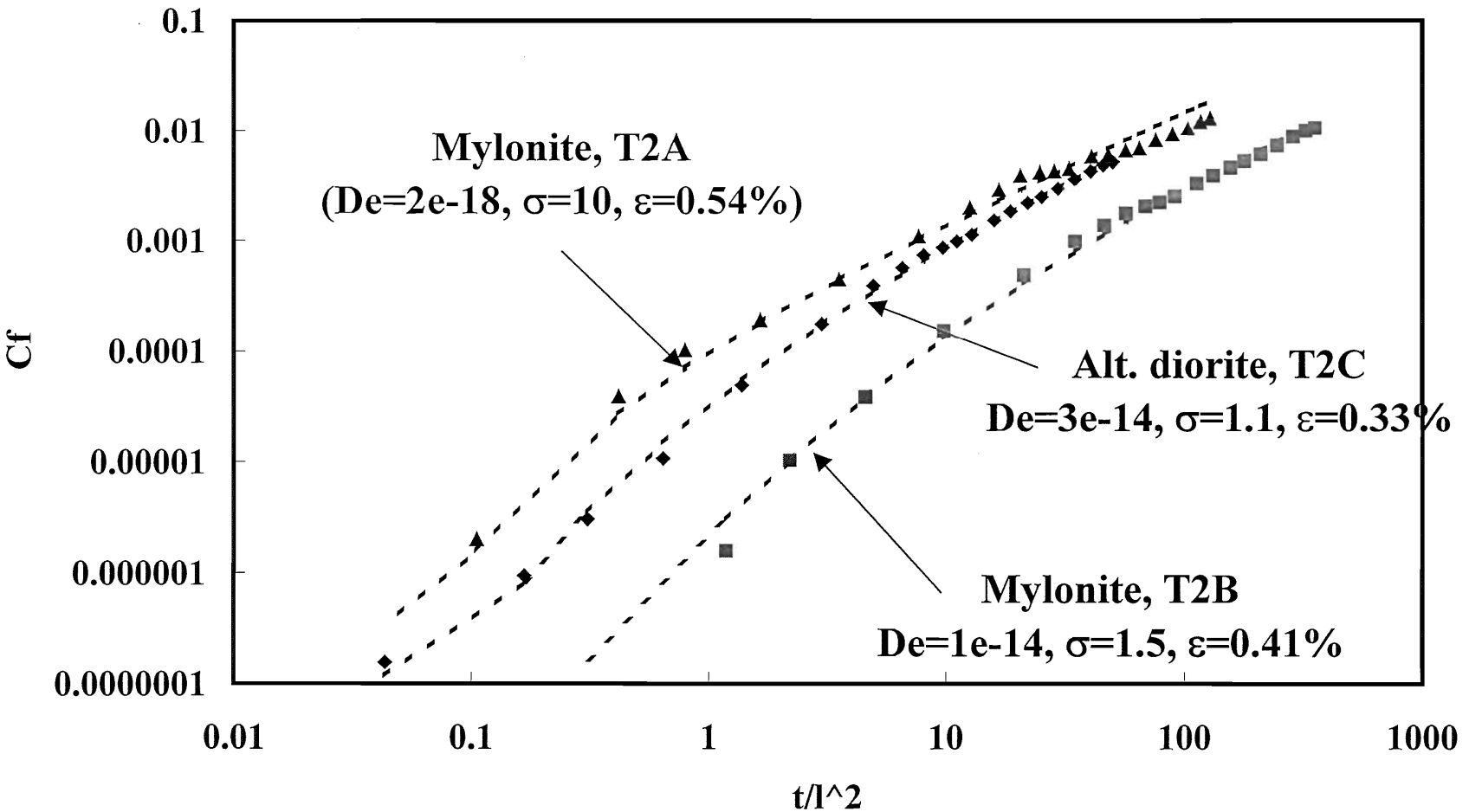
Fixed porosity, fitted De (m^2/s)



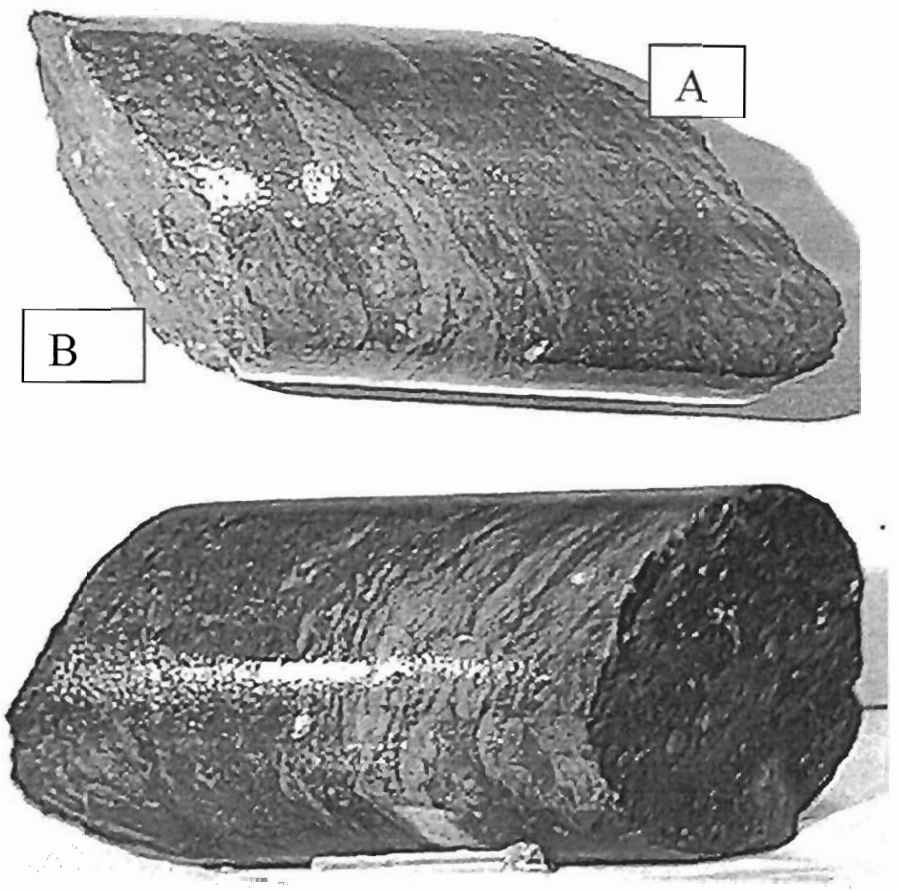
Fitting porosity and D_e (m^2/s)



Fixed porosity, fitted D_e (m^2/s) and σ_{De} (exp-units)



^{14}C-labelled MMA impregnation and polymerisation, KXTT3-core



Description of method

- 14C-labelled metamethylacrylate (MMA)is impregnated in the intact drillcore
- The impregnated drillcore is irradiated with high dose γ-radiation to polymerise the MMA
- Sawing of the impregnated rock sample is performed
- The porosity and porosity distribution is measured by autoradiography, followed by digital imaging

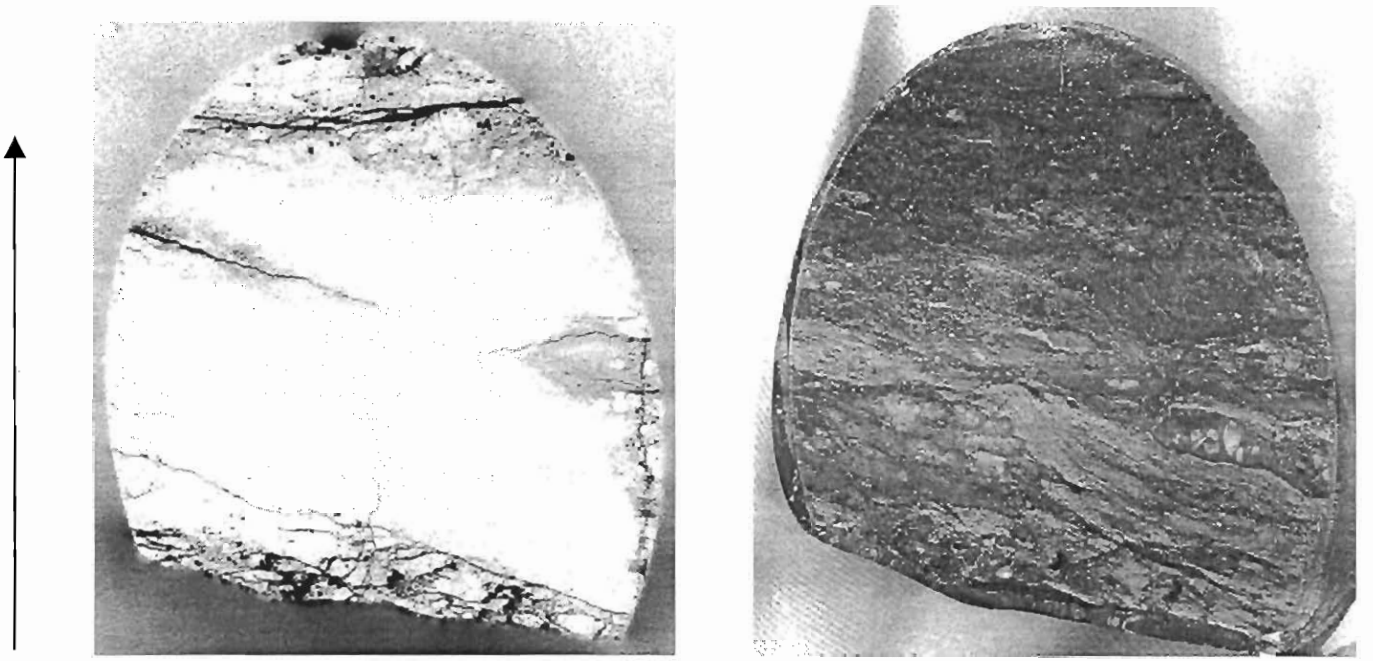
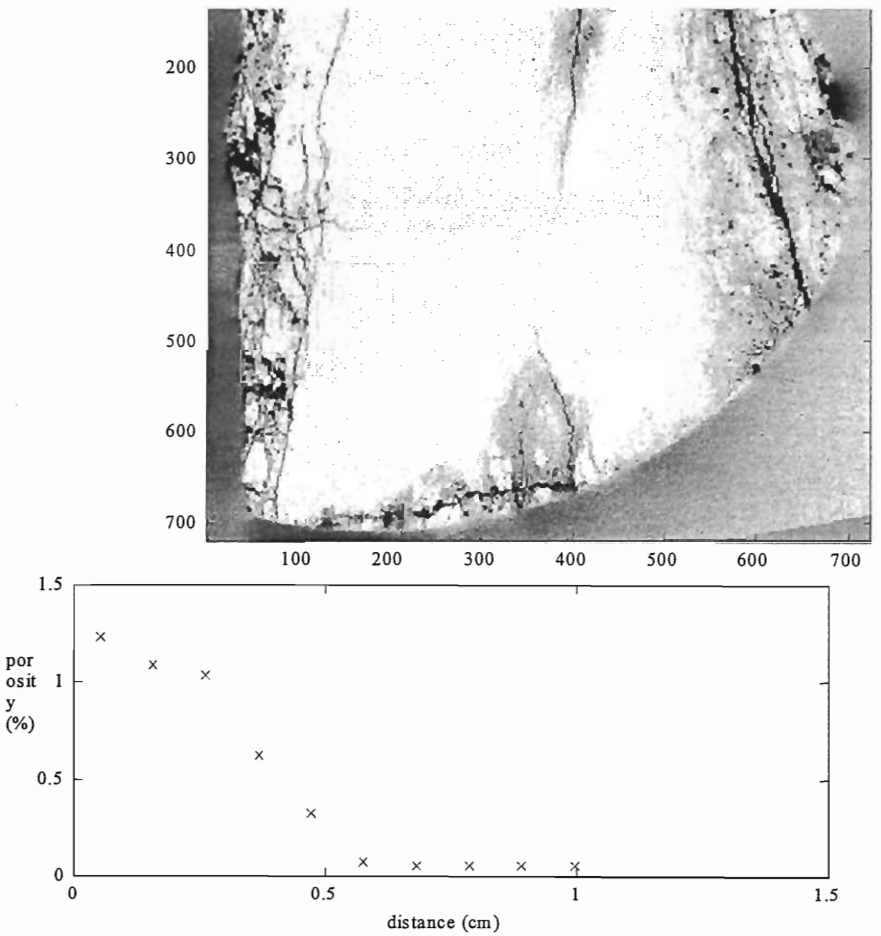


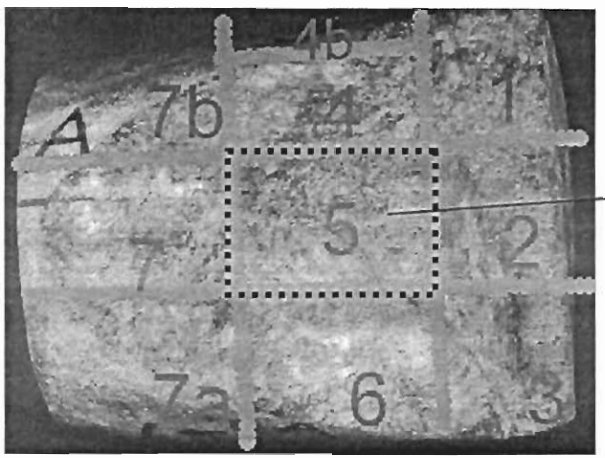
Figure 2. Autoradiographs (5 days exposure time) and corresponding photographs of sample T3'. Arrows are perpedicular to natural fracture surfaces.

Porosity profile



Penetration depth studies of KXTT1 diffusion cell slab

(Contact time: 1140d, Tracers remaining: Na-22, Cs-137, Ba-133)



Cutting and slicing for penetration depth studies

Photograph + Autoradiograph

Cutting

Penetration profile KXTT1, sample 5