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Progress Report

**IPR-99-22**

## Äspö Hard Rock Laboratory

### Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes

Proceedings from the 12<sup>th</sup> task force meeting  
at Gimo, Sweden, April 20-22, 1999

Part 1 of 3: Description and results compilation

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Svensk Kärnbränslehantering AB

September 1999

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**Äspö Hard Rock  
Laboratory**



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*Keywords:* Groundwater flow, solute transport, tracer test, fractured rock, underground laboratory, stochastic modelling, deterministic modelling.

This report concerns a study which was conducted for SKB. The conclusions and viewpoints presented in the report are those of the author(s) and do not necessarily coincide with those of the client.



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Groundwater Flow and Transport of Solutes

**Mansueto Morosini (ed.)**  
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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, 1<sup>st</sup> 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.

As of October 1998 ten foreign organizations in addition to SKB are participating in the Äspö HRL. These 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 (BMW), Germany, Empresa Nacional de Residuos Radiactivos (ENRESA), Spain and US DOE/Sandia National Laboratories.

## 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 12<sup>th</sup> Task Force meeting held at Gimo in Sweden April 20-22, 1999. It also constitutes a status report of the Task Force work. Task 1-3 have 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 1-1.

**Table 1-1. Modelling contributions.**

<b>Modelling Group</b>	<b>Task 4E</b> Explain STT1/1b	<b>Task 4F</b> Predict STT2	<b>Task 5</b> Predict 2900-3600m
ANDRA/ANTEA	n/a	n/a	n/a
ANDRA/CEA	n/a	submitted	n/a
ANDRA/ITASCA	n/a	n/a	n/a
BMW/BGR	submitted	submitted	submitted
CRIEPI		submitted	submitted
DOE/SANDIA	submitted	submitted	n/a
ENRESA/ULC	n/a	n/a	submitted
JNC/GOLDER	submitted	submitted	submitted
NAGRA/PSI	submitted	submitted	n/a
POSIVA/VTT	submitted	submitted	submitted
SKB/WRE	submitted	submitted	n/a
SKB/ChE	submitted	submitted	n/a

n/a : not applicable

Reports produced within the framework of the Äspö Task Force published since the previous 11<sup>th</sup> Task Force meeting are listed in the reference list.

## **3 Task 4 – Tracer retention and understanding experiments, 1<sup>st</sup> 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 which will constitute the necessary platform for subsequent, more elaborate experiments within TRUE.

#### **3.1.1 Introduction to the TRUE-1 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)
- 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

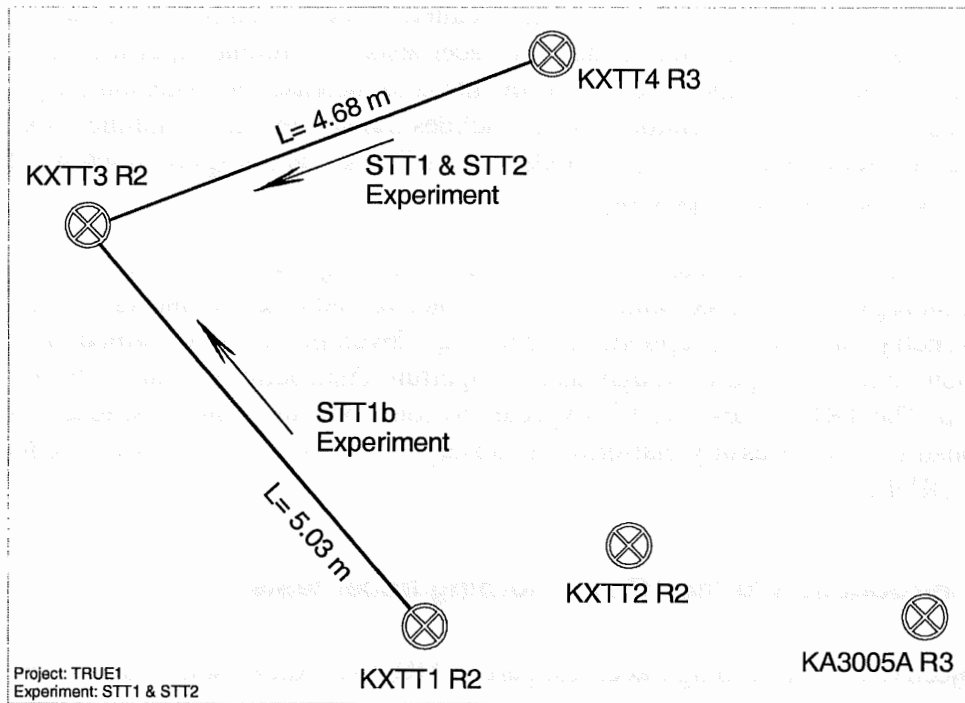


Figure 3-1 Borehole intersections with Feature A shown in the plane of the feature. Distances given in metres.

The STT1 test was performed in a radially converging flow geometry with injection in borehole KCTT4 and withdrawal in borehole KXTT3. The test is performed at pumping rate of 0.4 mL/min and involved a modified tracer injection with a finite pulse of 4 hours. Test started in the middle of July 1997 injection of the conservative tracers Uranine and HTO but also with weakly to moderately sorbing tracers  $^{22}\text{Na}$ ,  $^{85}\text{Sr}$ ,  $^{86}\text{Rb}$ ,  $^{47}\text{Ca}$ ,  $^{133}\text{Ba}$  and  $^{137}\text{Cs}$ .

In addition, a new complementary injection, STT1b, was performed in order to obtain data from a different flow path than STT1, see Figure 3-1.

### 3.2 Experiment with sorbing tracers – Task 4E and 4F

The TRUE-1 experimental team presented results from the STT-2 experiment (Task 4F), these are included in Appendix A. The modelling teams presented their evaluation of the STT1/1b experiment (Task 4E) and predictive modelling of the STT2 experiment.

Predictive modelling results for the STT2 experiment are attached in Appendix B.2 and a comparative compilation of these modelling results is found in Appendix B.1.

The STT2 experiment is performed in a dipole configuration where tracers are injected in KXTT4 R3 and pumping takes place in KXTT3 R2 with 0.201L/min situated 4.7m away in feature A (Figure 3-1). A cocktail of twelve different tracers (Table 3-1) were injected simultaneously as a finite pulse with a duration of 4 hours. Tracers were recovered in-line with a HpGe detector. A thorough description of the experiment and preliminary evaluation of results is reported by Andersson et al (1999).

**Table 3-1 STT-2 Injected tracers**

<b>Conservative tracers</b>	<b>Radioactive sorbing tracers</b>
Uranine, HTO, $^{82}\text{Br}$	$^{22}\text{Na}$ , $^{47}\text{Ca}$ , $^{42}\text{K}$ , $^{85}\text{Sr}$ , $^{86}\text{Rb}$ , $^{99\text{m}}\text{Tc}$ , $^{131}\text{Ba}$ , $^{133}\text{Ba}$ , $^{134}\text{Cs}$

### 3.3 Evaluation of STT1b predictions and Predictive modelling of STT2

The evaluation of the predictive modelling done on STT1/1b is reported together with the prediction for STT2. Report titles and presenter are listed in Table 3-1 while the actual reports are compiled in Appendix B3.

**Table 3-2 Task 4 E and 4F technical presentations**

<b>Title</b>	<b>Organisation</b>	<b>Presenter</b>
Modelling of sorption behaviour of radioactive tracer in feature A using different conceptual models	BMWi	H. Shao, BGR
Modelling of STT1 tracer test and Predictive computations of STT2	ANDRA	C. Grenier, CEA
Modelling of STT1b tracer tests and Prediction of STT2 tracer tests	SKB	L. Moreno, KTH-KAT
Evaluation of STT1 and prediction of STT2	SKB	J-O. Selroos, SKB (TRUE Team)
Analysis of the STT1 and STT1b tests and Predictions of the breakthrough times in the STT2 test	POSIVA	A. Poteri, VTT
STT2 predictions	JNC	W. Dershowitz, Golder
Numerical analysis with FEGM/FERM for TRUE-1 sorbing tracer tests.	CRIEPI	Y. Tanaka, CRIEPI
Estimation of STT-1b and STT1 and Blind predictions of the STT2 tracer tests with multiple rates of mass transfer.	DOE/Sandia	S. McKenna, Sandia
Analysis of STT1b-What have we learned?	NAGRA	W. Heer, PSI
Results of STT2 experiment	SKB	P. Andersson, Geosigma

### 3.4 Results of the STT2 experiment

The experimental results and framework are presented in Appendix A. Some of observations related to the experiment are summarised below:

- Sorption on borehole walls can be observed, from plots of injection concentration
- In-line measurements gives better description than samples
- Second peak after exchange procedure due to stagnant zones in the injection section
- Mass flux calculations based on Uranine data
- Breakthrough of all tracers except Tc monitored in pumping borehole
- Breakthrough of K only a few points due to short half-life
- Tracer arrival  $t_5$  vary between 11 (Uranine) to 1528 hours (Cs)
- High recovery (>80%) for Uranine, HTO, Br, Na, (Ca)
- Low recovery (<20%) for Cs

### 3.5 Performance measures for Task 4F

Results presented by the modelling teams for the modelling of Task 4F in the appendices B.3 adhere to performance measures previously agreed upon, as presented in this section.

The basic performance measures are:

- Steady-state drawdown,  $s$  [m], in the injection and extraction sections.
- Breakthrough curves (mass flow and cumulative mass) including explicit listing of  $t_5$ ,  $t_{50}$ , and  $t_{95}$  [hr] for both a dirac pulse input and measured input.
- Mass recovery,  $F=M_{\text{ext}}/M_{\text{inj}}$  [-], for both pulse input and measured input mass.

The measures are calculated for a single deterministic realization, or for every realization of generated stochastic Monte Carlo realizations. In the latter case, 5, 50 and 95 percentiles of the measures are to be calculated, i.e.,  $s_{(5\%)}$ ,  $s_{(50\%)}$ ,  $s_{(95\%)}$ ,  $t_{5(5\%)}$ ,  $t_{5(50\%)}$ ,  $t_{5(95\%)}$ ,  $t_{50(5\%)}$ ,  $t_{50(50\%)}$ ,  $t_{50(95\%)}$ ,  $t_{95(5\%)}$ ,  $t_{95(50\%)}$ ,  $t_{95(95\%)}$ ,  $F_{(5\%)}$ ,  $F_{(50\%)}$ ,  $F_{(95\%)}$ . Median breakthrough curves are also to be presented in the latter case.

The time of termination of monitoring ( $t_t$ ) in the extraction hole, for each tracer if applicable, will be provided by the Task Force secretariat. Mass recovery is to be calculated at this time.

Full recovery is defined as  $F=M_{\text{ext}}/M_{\text{inj}}=1$  at time  $t_{100}$ ). Hence, if e.g. a calculated recovery of less than 95% is obtained at the end time of the simulation,  $t_{95}$  should not be provided. The appropriate simulation time is chosen by the individual modellers. However, the simulation time is to be set equal or longer than the time of termination of monitoring ( $t_t$ ) in the extraction hole, cf. Figure 1.

Both breakthroughs (mass flow [1/hr] and cumulative mass [-]) are to be plotted normalized to the injected mass (i.e. normalized total mass=1) with time units [hr].

A logarithmic time axis should be used with a decade length of 0.05 m. The normalized mass flow axis should be logarithmic with an axis length of 0.12 m, using 0.02 m per decade. The normalized cumulative mass axis should be linear with an axis length of 0.12 m.



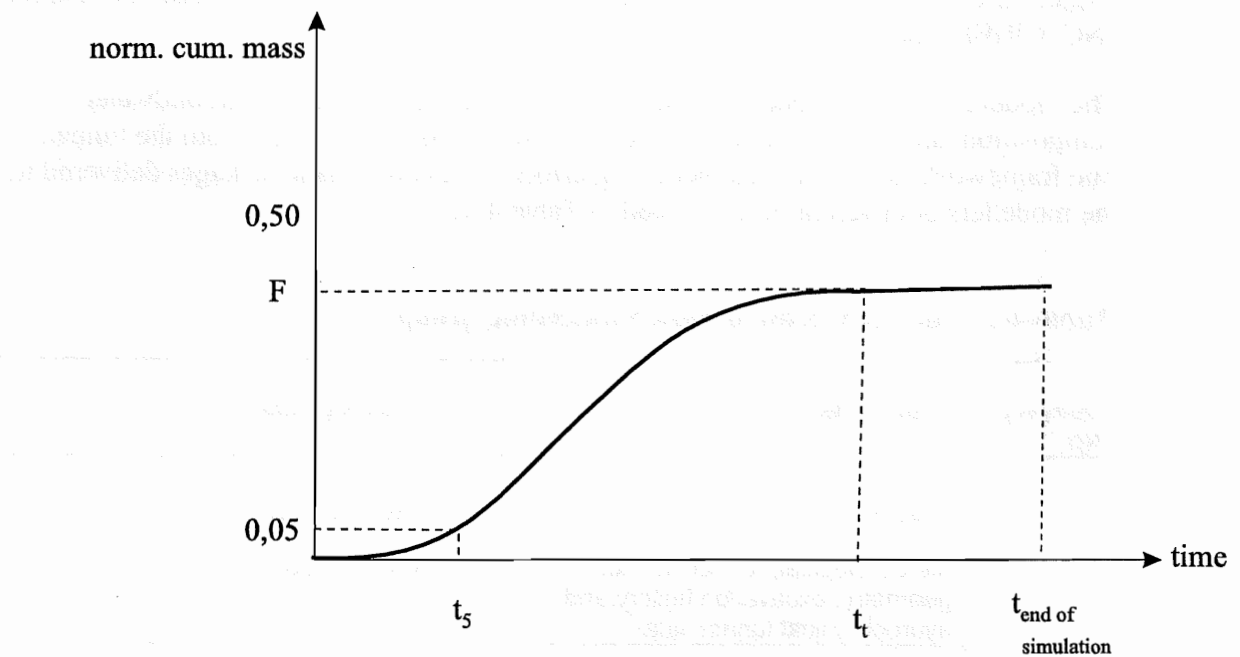
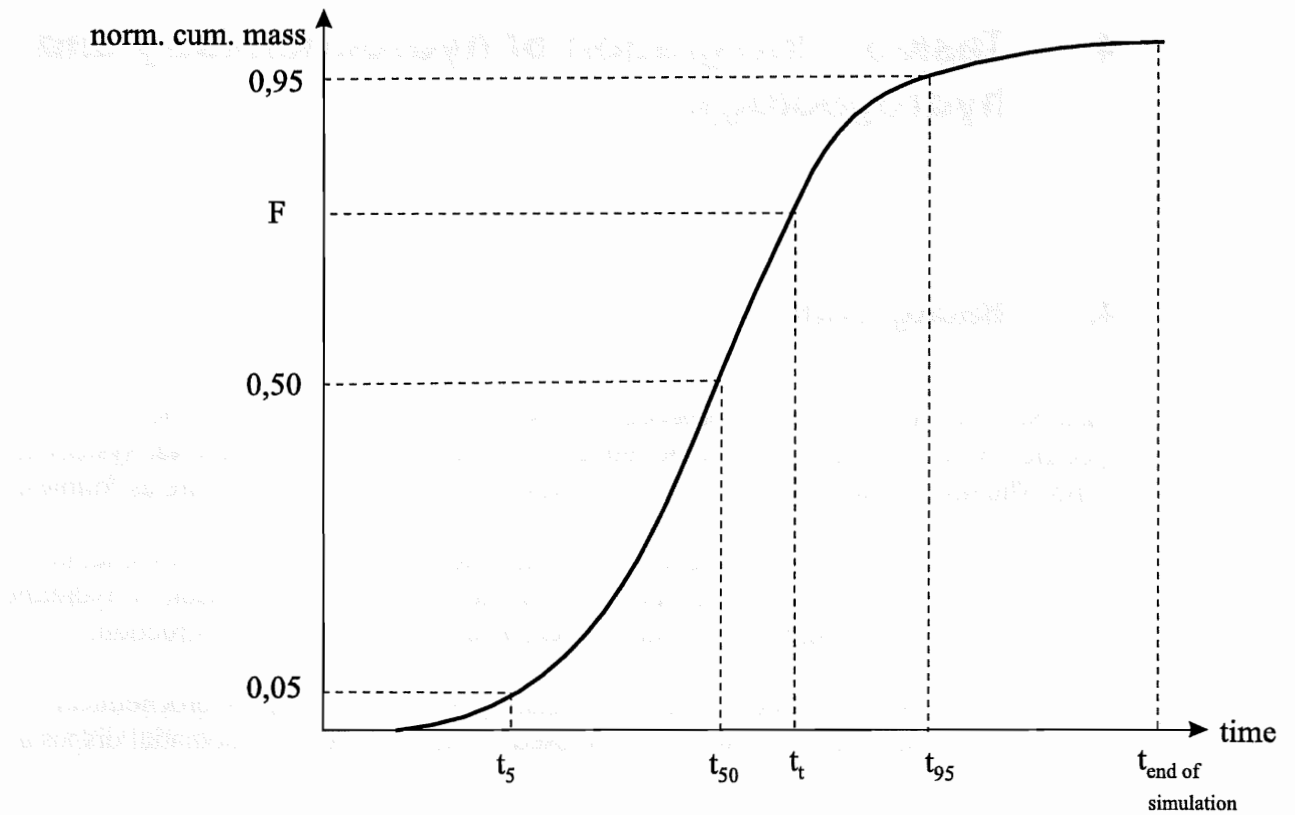


Figure 3-2 Two examples of  $t_5$ ,  $t_{50}$ ,  $t_{95}$ , and mass recovery  $F$  for a single deterministic or stochastic realization (pulse or measured input function).

## 4 Task 5 – Integration of hydrochemistry and hydrogeology.

### 4.1 Background

Task No 5 is a hydrological-hydrochemical model assessment exercise which specifically studies the impact of the tunnel construction on the groundwater system at Äspö. The task definition has been successively refined. The objectives are as follows:

- 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 which 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 composition 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 as listed in Table 4-1.

**Table 4-1 Data deliveries to Task 5 modelling groups**

Delivery No	Type of data	Delivery data
1	Hydrochemical data	February 1998
2	Meteorological, tunnel and zone geometry, excavation history and hydrochemical tunnel data	March 1998
3	Piezometric levels and salinity in borehole sections, borehole coordinates	March 1998
4	Hydrochemical initial and boundary conditions	June 1998
5	Topographical data for the site	August 1998
6	Hydraulic interference tests including LPT2 (Task 1&3 deliveries)	November 1998

7	Update on hydrochemical initial and boundary conditions	October 1998
8	Performance measures and control points	November 1998
9	Water flow into the Äspö tunnel	February 1999

## 4.2 Predictive modelling 2900-3600m

Task 5 modelling results were presented by ENRESA, BMWi/BGR, CRIEPI, JNC/Golder, POSIVA/VTT, SKB/CFE and SKB/Intera. A list of the presenter along with the titles is listed in Table 4-2. Their modelling reports are compiled in Appendix C.

Since ANDRA recently joint Task 5 they could not present any results. They have included three modelling teams with different modelling concept approaches: ITASCA with the discrete feature, CEA with stochastic continuum and ANTEA with the double porosity approach.

**Table 4-2 Task 5 technical presentations**

Title	Organisation	Presenter
Presentation of chemistry data	SKB	M. Laaksoharju, Intera
Modelling the composition of the groundwater leaking into the Äspö HRL	SKB	U. Svensson, CFE
Hydraulic DFN modelling of Task 5	JNC	W. Dershowitz, Golder
The proportion of water from different sources in the water drained from the Äspö HRL	BMWi	L. Liedtke, BGR
Executive summary of modelling 2900-3600m	POSIVA	E. Kattilakoski, VTT
Preliminary application of FEGM/FERM to Task 5	CRIEPI	T. Hasegawa, CRIEPI.
Numerical modelling of flow and transport during the tunnel construction of Äspö HRL.	ENRESA	J. Molinero, ULC
Prediction of water composition using M3	SKB	M. Laaksoharju, Intera

## 5 References

**Andersson, P., Wass E., Byegård, J., Johansson, H., Skarnemark, G. (1999).** Tracer tests with sorbing tracers, STT2: Experimental description and evaluation. TRUE1st stage tracer test programme. Äspö Hard Rock Laboratory. SKB International Progress Report IPR-99-15.

**Elert, M. (1999).** Evaluation of modelling of the TRUE-1 radially converging and dipole tests with conservative tracers. Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes, Task 4C and 4D. SKB Technical Report TR 99-04.

**Mahara, Y., Igarashi, T., Miyakawa, K., Kiho, K., Tanaka, Y., Hasegawa, T. (1998).** Dynamic changes in groundwater conditions caused by tunnel construction at the Äspö Hard Rock Laboratory, Sweden. Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes. SKB International Cooperation Report ICR 98-04.

**J-O. Selroos and V. Cvetkovic (1998).** Prediction of TRUE-1 radially converging and dipole tracer tests. Task 4C and 4D. Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes. SKB International Cooperation Report ICR 98-07.

**Anders Ström (1999).** Issue Evaluation Table 1997/1998. Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes. SKB International Cooperation Report ICR 98-05.

**W. Worraker, D. Holton, K. A. Cliffe (1998).** Modelling TRUE-1 (RC-1) tracer tests using a heterogenous variable aperture approach. Task 4C. Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes. SKB International Cooperation Report ICR 98-06.

## **Appendix A - Results of the STT2 experiment**



## **RESULTS FROM THE STT-2 TRACER EXPERIMENT**

**Presentation at the 12th Meeting of the Task Force on Modelling  
of Groundwater Flow and Transport of Solutes**

**Gimo City, Sweden  
20-22<sup>nd</sup> April 1999**

**Peter Andersson  
GEOSIGMA AB**

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**Brief description of methodology and equipment**

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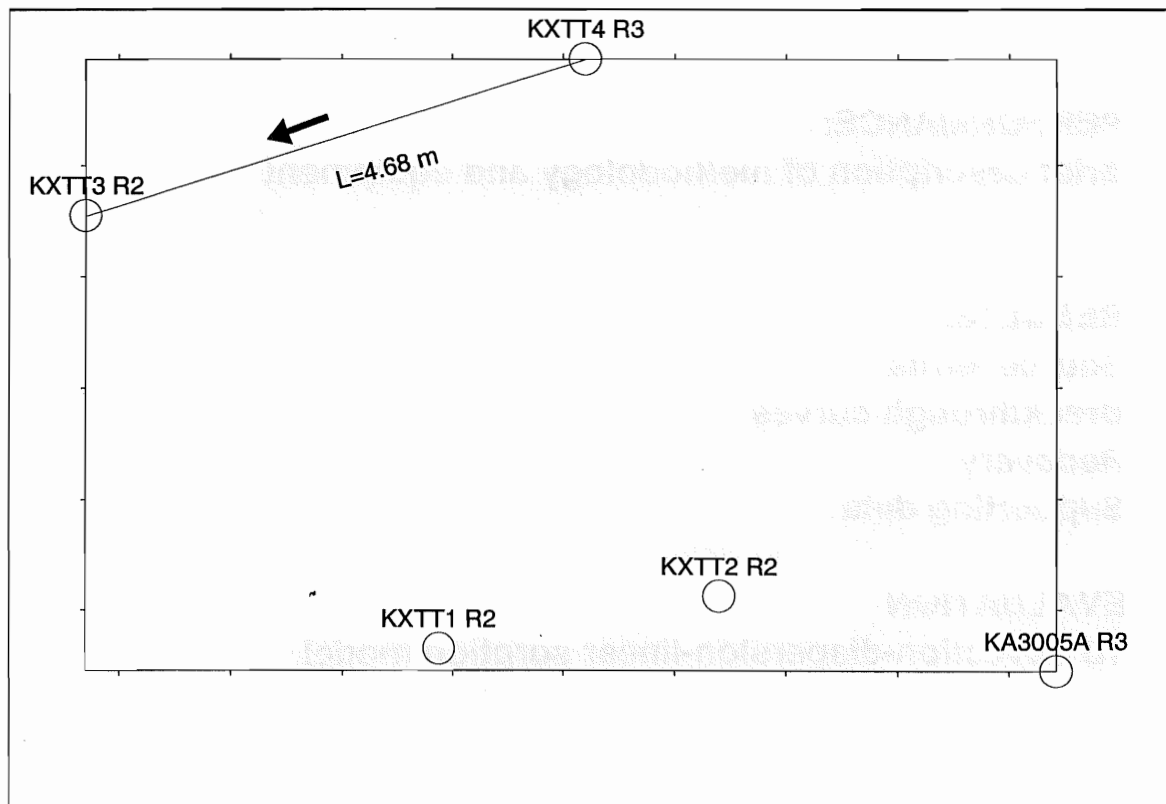
**1D advection-dispersion-linear sorption model**

## PERFORMANCE

- Radially converging flow, injection in KXTT4 R3, pumping in KXTT3 R2
- Simultaneous injection of 12 different tracers, 3 conservative (Uranine, HTO, Br) and 9 sorbing radioactive isotopes (Na, Ca, Sr, K, Tc, Rb, Ba, Cs)
- Injection performed as a finite pulse (4 hours) by exchange of tracer solution with water (same procedure as STT-1)
- In-line measurement of source term for radioactive tracers (HpGe detector)

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### EXPERIMENTAL GEOMETRY STT-2 (plane view of Feature A)





## STT-2 SOURCE TERMS

- Sorption on borehole walls can be observed
  - In-line measurements gives better description than samples
  - Second peak after exchange procedure due to stagnant zones in the injection section
  - Mass flux calculations based on Uranine data
- 

## HYDRAULIC HEAD AND DRAWDOWN

- Hydraulic head and drawdown not the same as RC-1 and PDT-2 (same pumping rate)
- Head difference T4R3→T3R2 = 5.5-7.5 m (2.8 m and 2.3 m during RC-1 and PDT-2)
- Pumping rate constant 0.201 l/min
- Electrical conductivity slightly decreasing from 1180 to 1160 mS/m

## HYDRAULIC HEAD AND DRAWDOWN

Borehole	KXTT1 R2	KXTT2 R2	KXTT3 R2	KXTT4 R3	KA3005A R3
H0 (m)	-53.4	-53.8	-52.7	-52.6	-54.1
H1 (m)	-55.4	-59.2	-59.4	-53.9	-55.3
Drawdown (m)	2.0	5.4	6.7	1.3	1.2
Head diff (m)	4.0	0.2	0	5.5	4.1

## RESULTS

- Breakthrough of all tracers except Tc monitored in pumping borehole
- Breakthrough of K only a few points due to short half-life
- Tracer arrival  $t_s$  vary between 11 (Uranine) to 1528 hours (Cs)
- High recovery (>80%) for Uranine, HTO, Br, Na, (Ca)
- Low recovery (<20%) for Cs

## NUMERICAL MODELLING

- 1D Advection-dispersion-linear sorption model (same as in earlier tests)
- Automatic parameter estimation by non-linear least-square regression including error estimates
- Discretization of source term in 50 time steps
- Using standard error ( $1/s^2$ ) as weight for each data point
- Modelling in two steps, first conservative tracers, then simultaneous run with conservative and sorbing tracers
- Parameters determined from step 1: mean travel time,  $t_m$ , dispersivity,  $D/v$ , proportionality factor. Additional parameters determined from step 2: retardation coefficient,  $R$ , relative inj. concentration,  $f_c$

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

Test*	Q (l/min)	$\Delta h$ (m)	R (%)	$D/v$ (m)	$K_{fr}$ (m/s)	$b$ (m)	$\theta_k$
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** 0.46***	$3.4 \cdot 10^{-4**}$ $1.0 \cdot 10^{-4***}$	$1.3 \cdot 10^{-3**}$ $4.5 \cdot 10^{-3***}$	$1.1 \cdot 10^{-3**}$ $4.0 \cdot 10^{-3***}$

\* Pumping increased during experiment

Evaluated parameters for the conservative tracers in STT-2 using PAREST (advection-dispersion model). Separate runs for each tracer. Values within brackets are standard errors in percent.

\*\* Flow path #1 \*\*\* Flow path #2

Tracer	Mean velocity, $v$ (m/s)	Mean travel time, $t_0$ (h)	Dispersivity, $D/v$ (m)	Proportionality factor, $F$
Uranine	$1.74 \cdot 10^{-4}$ (1) *	7.5 (1) *	0.35 (3) *	$6.2 \cdot 10^{-4}$ (1) *
	$5.05 \cdot 10^{-5}$ (1) **	25.8 (1) **	0.46 (3) **	$1.4 \cdot 10^{-3}$ (1) **
HTO	$1.78 \cdot 10^{-4}$ (2) *	7.3 (2) *	0.25 (4) *	$3.1 \cdot 10^{-4}$ (6) *
	$4.39 \cdot 10^{-5}$ (2) **	29.6 (2) **	1.2 (7) **	$1.6 \cdot 10^{-3}$ (1) **
Br-82	$1.68 \cdot 10^{-4}$ (1) *	7.7 (1) *	0.32 (3) *	$4.9 \cdot 10^{-4}$ (2) *
	$4.746 \cdot 10^{-5}$ (1) **	27.4 (1) **	0.54 (5) **	$1.3 \cdot 10^{-3}$ (2) **

\* Flow path #1

\*\* Flow path #2

**Evaluated parameters from PAREST (Advection-dispersion-linear sorption model). Simultaneous run Uranine and sorbing tracer.**

Tracer	v (m/s)	t <sub>0</sub> (h)	D/v (m)	F	R	f <sub>c</sub>
Uranine	1.74·10 <sup>-4</sup>	7.5	0.35	6.2·10 <sup>-4</sup>	1	1
	5.05·10 <sup>-5</sup>	25.8	0.46	1.4·10 <sup>-3</sup>		
Na-22	2.06·10 <sup>-4</sup>	6.3	0.38	3.6·10 <sup>-4</sup>	1.54	0.82
	5.08·10 <sup>-5</sup>	25.6	1.5	1.8·10 <sup>-3</sup>		
Ca-47	1.74·10 <sup>-4</sup>	7.5	0.35*	6.2·10 <sup>-4</sup>	2.34	0.70
	5.04·10 <sup>-5</sup>	25.8	0.46*	1.4·10 <sup>-3</sup>		
Sr-85	7.42·10 <sup>-5</sup>	17.5	3.0*	1.9·10 <sup>-3</sup>	2.62	0.74
	1.19·10 <sup>-5</sup>	110	6.1*	6.5·10 <sup>-4</sup>		
Ba-131	1.74·10 <sup>-4</sup>	7.4	0.34	6.1·10 <sup>-4</sup>	6.96	0.44
	5.02·10 <sup>-5</sup>	25.9	0.48	1.4·10 <sup>-3</sup> *		
Ba-133	1.76·10 <sup>-4</sup>	7.4	0.33	6.0·10 <sup>-4</sup>	14.7	0.55
	5.04·10 <sup>-5</sup>	25.8	0.51	1.4·10 <sup>-3</sup>		
Rb-86	1.74·10 <sup>-4</sup>	7.5	0.34	6.2·10 <sup>-4</sup>	18.4	0.44
	5.04·10 <sup>-5</sup>	25.8	0.46	1.4·10 <sup>-3</sup>		
Cs-134	1.46·10 <sup>-4</sup>	8.9	0.72	8.1·10 <sup>-4</sup>	140	0.37
	4.70·10 <sup>-5</sup>	27.7*	0.36	1.2·10 <sup>-3</sup>		

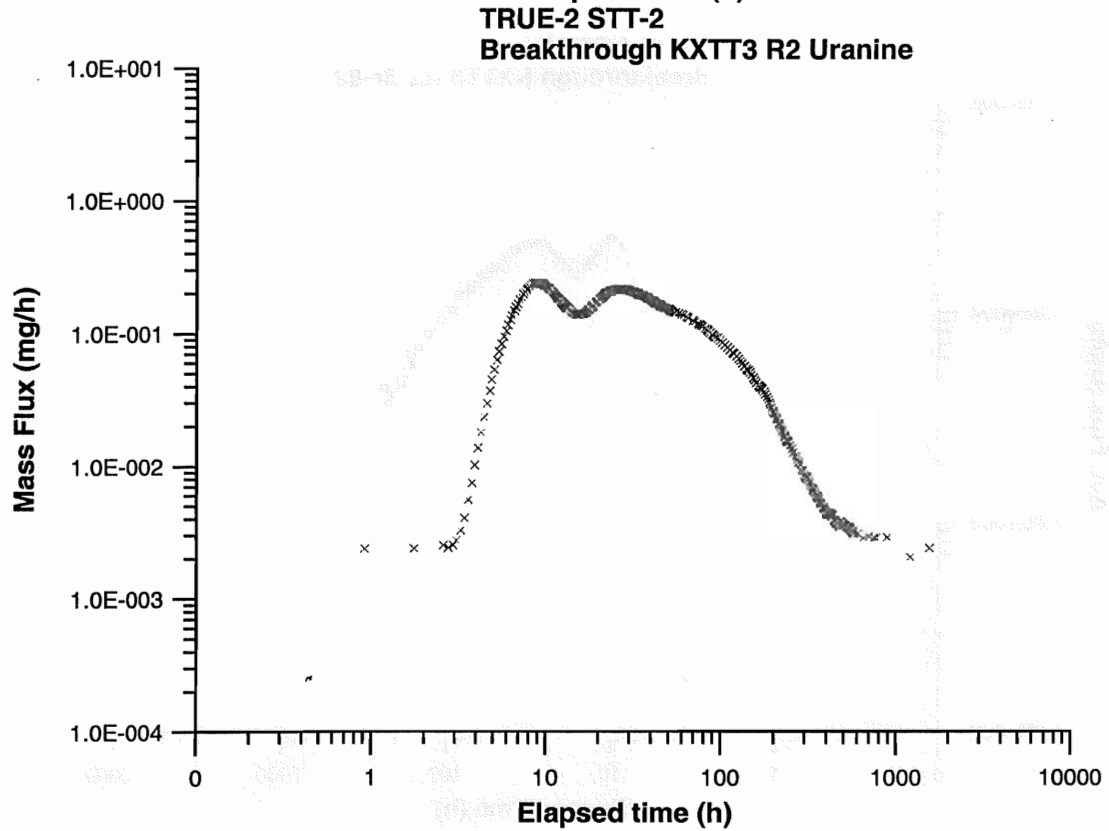
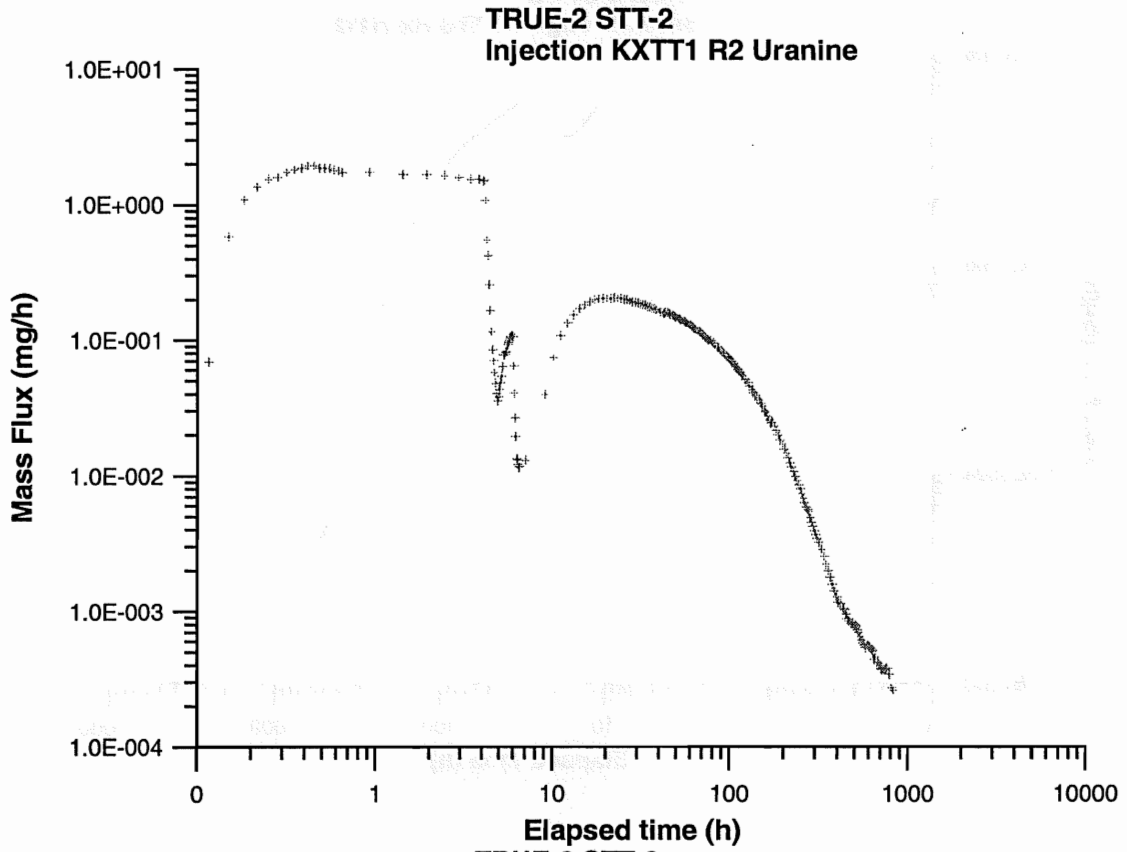
## MODELLING RESULTS

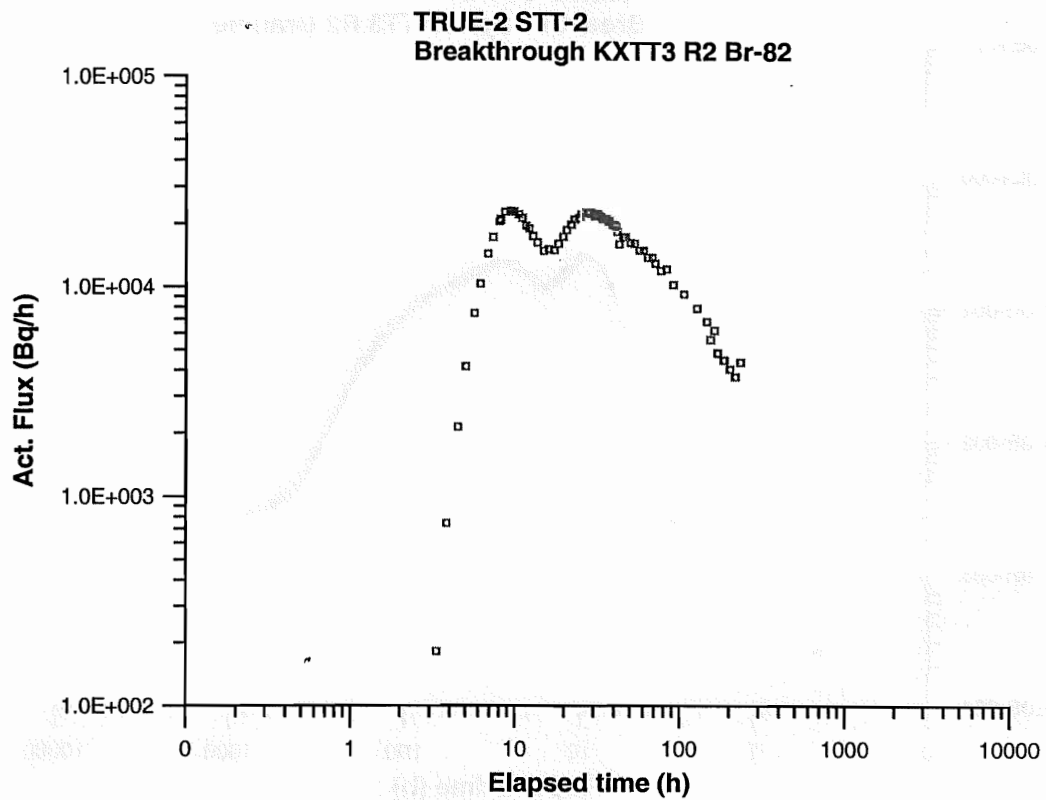
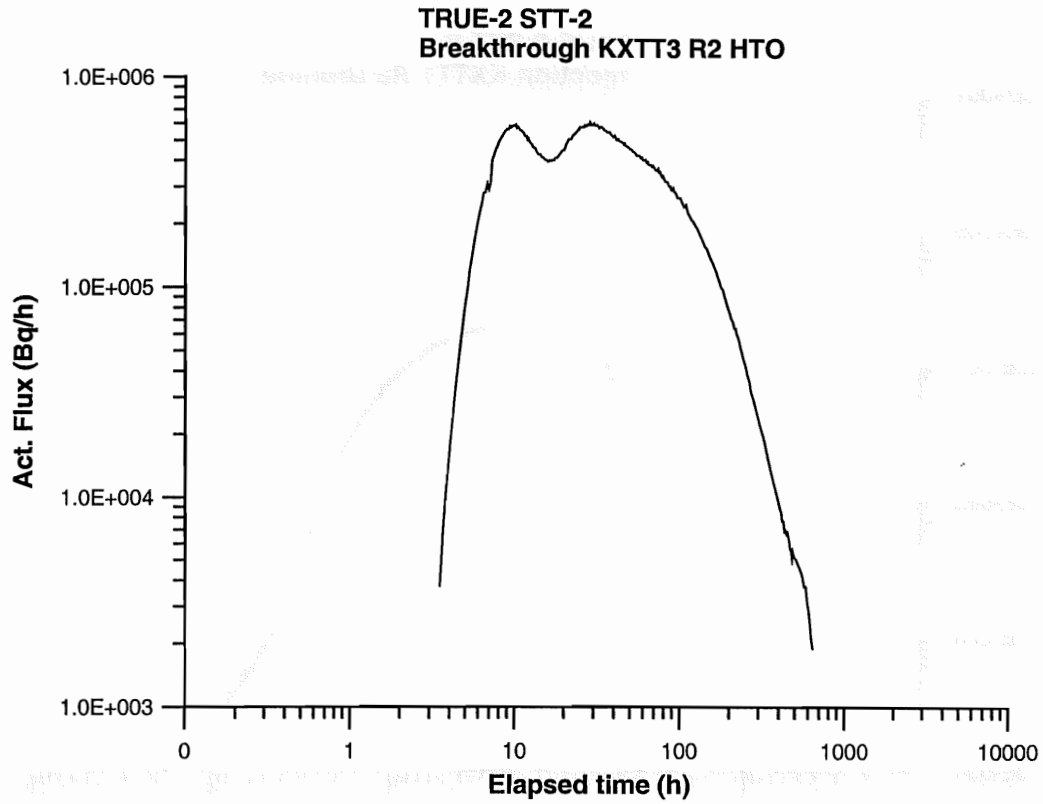
- Two flow paths needed to get acceptable model fit
- Consistent with earlier interpretation of dual flow paths to as an explanation for extremely high dispersivity
- Good fits to experimental data for conservative tracers, Na and Sr using linear sorption
- Not possible to fit Rb, Ba and Cs with linear sorption only
- Retardation coefficients vary between 1.5 (Na) and 140 (Cs) similar to STT-1 and STT-1b

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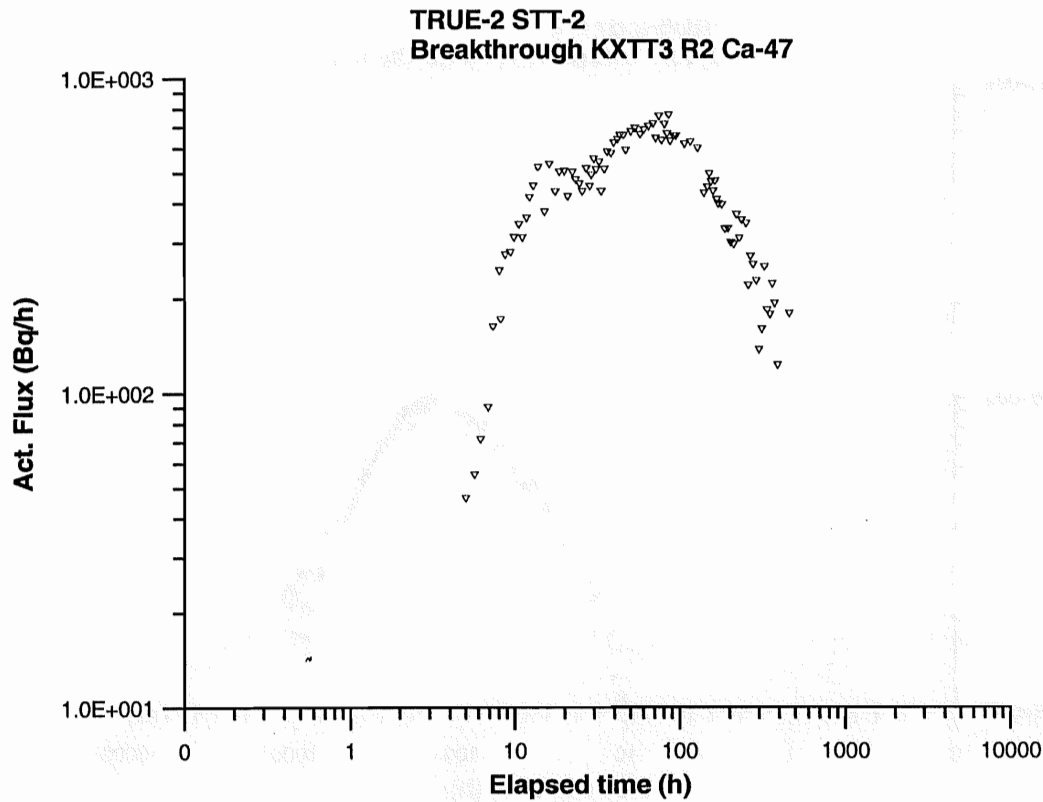
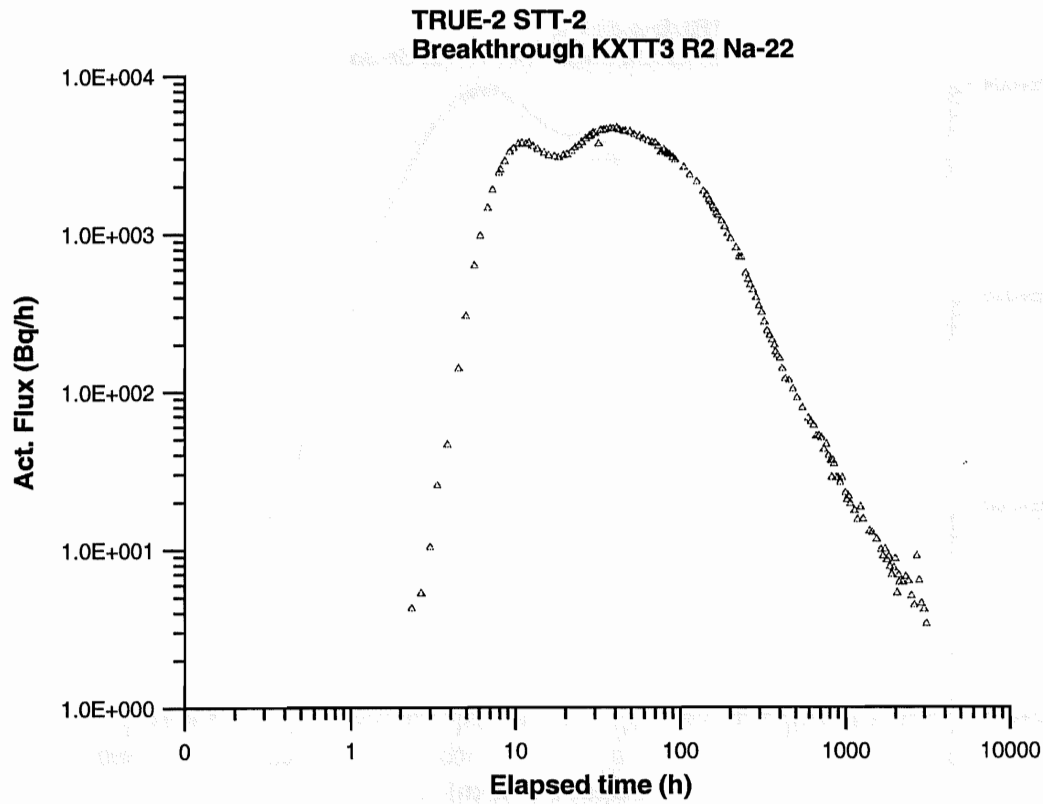
Comparison of linear retardation coefficients determined from lab and in situ (STT-1, STT-1b and STT-2)

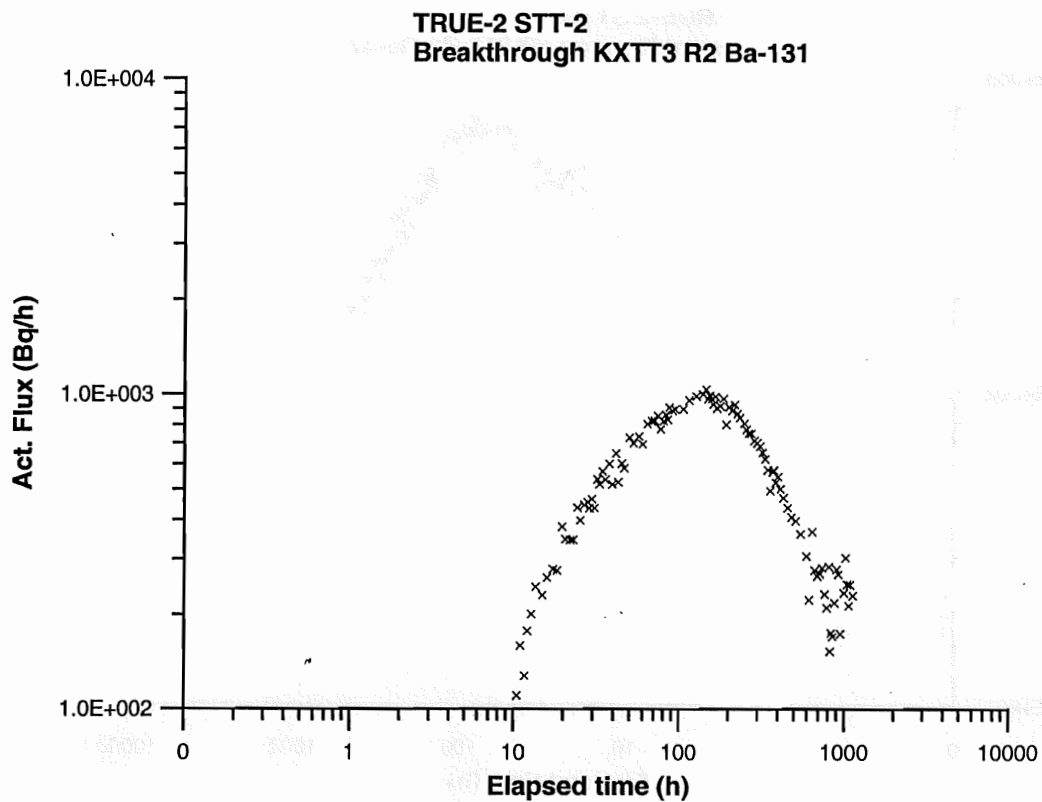
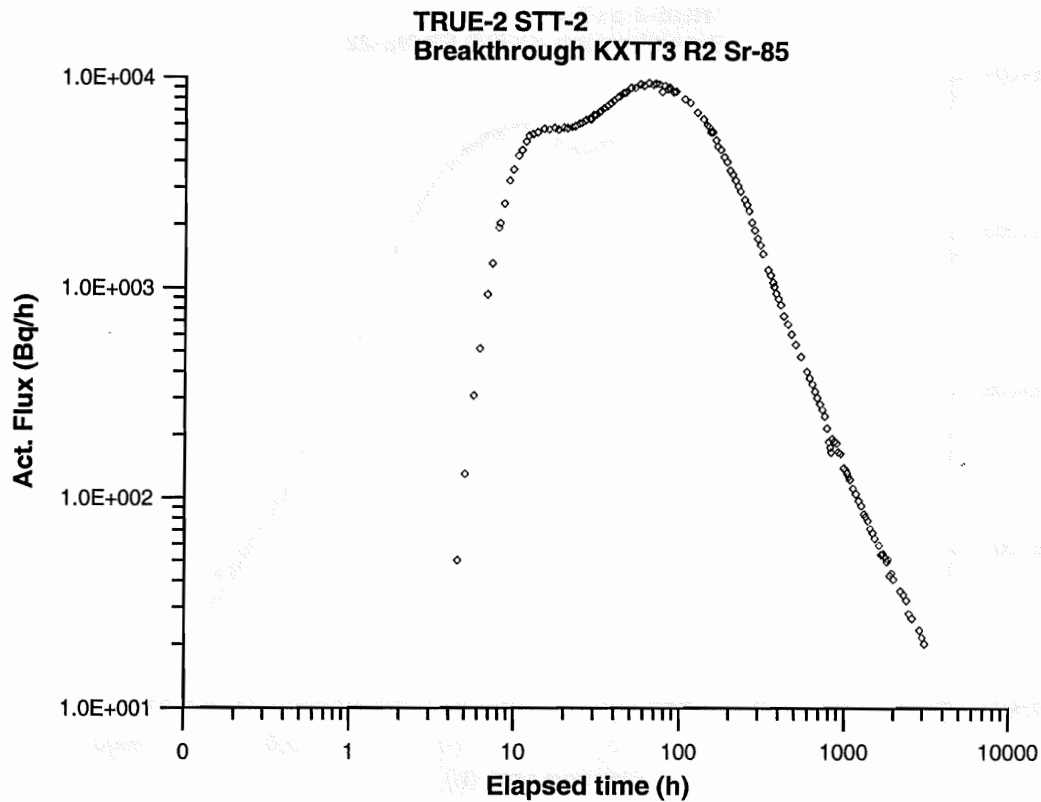
Tracer	R (lab)*	R (STT-1)	R (STT-2)	R (STT-1b)
Na	1.001-1.01	1.5	1.5	1.4
Ca	1.006-1.06	1.6	2.3	-
Sr	1.008-1.04	2.1	2.6	1.9
K	-	-	-	2.8
Ba	1.08-2.2	8.6	7-14	-
Rb	1.12-3.0	15	18	17
Co	-	-	-	57
Cs	2-21	69	140	118



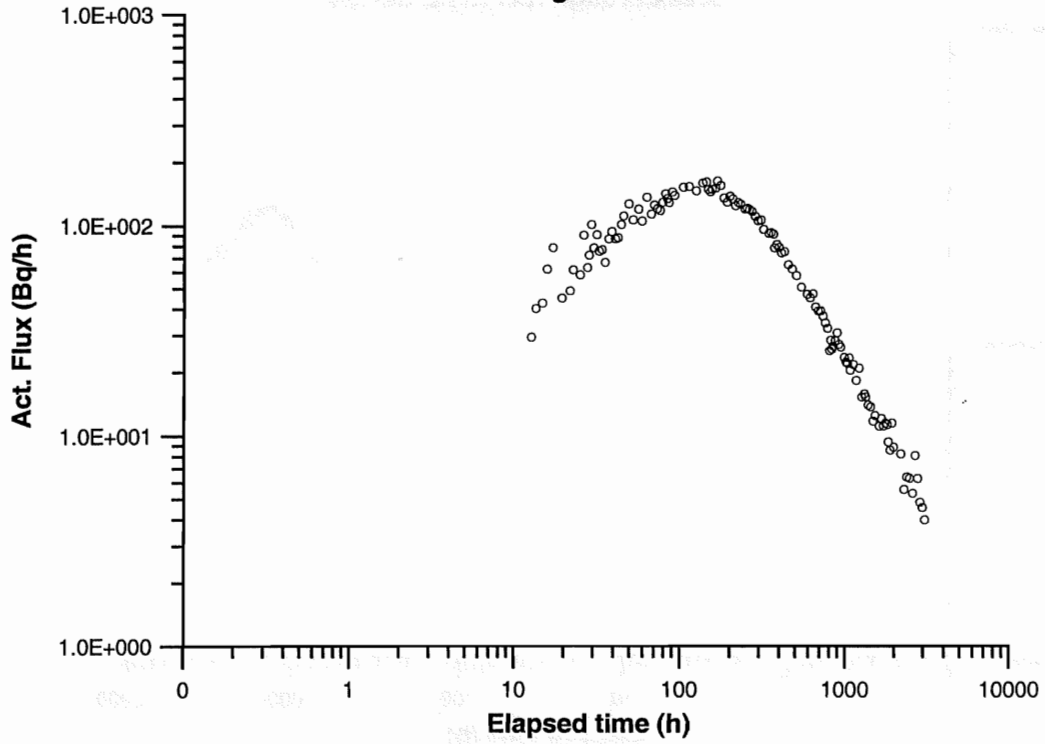




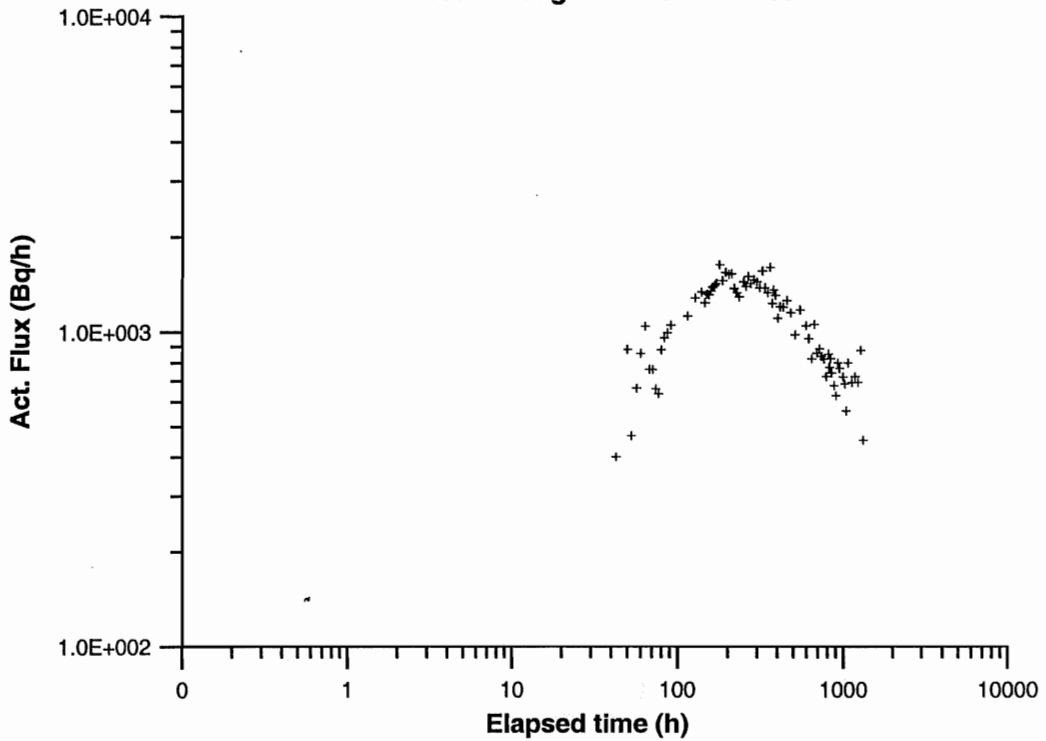




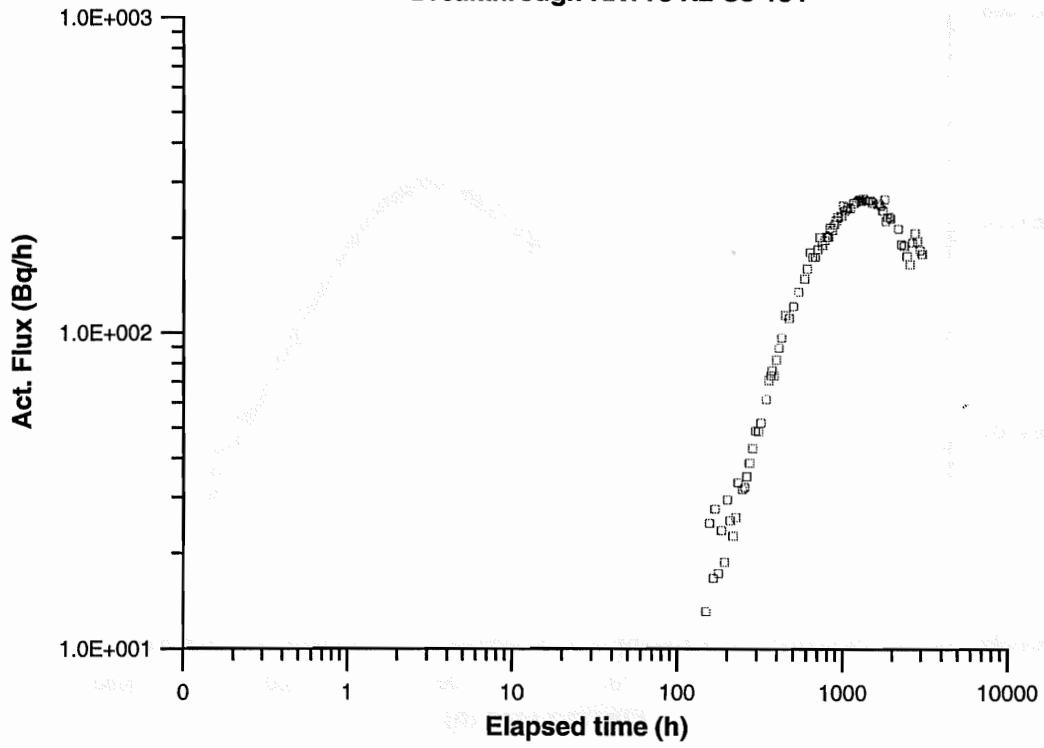
**TRUE-2 STT-2  
Breakthrough KXTT3 R2 Ba-133**



**TRUE-2 STT-2  
Breakthrough KXTT3 R2 Rb-86**



TRUE-2 STT-2  
Breakthrough KXTT3 R2 Cs-134



## **Appendix B - Task 4F modelling results**

### **B.1 Comparison of STT2 modelling results**

### **B.2 Evaluation of Task 4C and 4D**

- Evaluation of Task 4C and 4D. M Elert (SKB/Kemakta)
- Dirac modelling of STT1 & STT1b. M Elert (SKB/Kemakta)

### **B.3 Contributions of modelling results of Task 4E and 4F**

- Modelling of sorption behaviour of radioactive tracer in Feature A using different conceptual models. Hua Shao (BMBF/BGR)
- Modelling of STT1 tracer test and Predictive computations of STT2. C Grenier (ANDRA/CEA)
- Evaluation of STT1 and Prediction of STT2. J-O Selroos (SKB/WRE)
- Analysis of STT1 and STT1b tests and Predictions of the breakthrough times in the STT2 test. A Poteri (POSIVA/VTT)
- STT2 predictions. W Dershowitz (JNC/Golder)
- Numerical analysis with FEGM/FERM for TRUE-1 sorbing tracer tests. Y Tanaka, T Igarashi, M Kawanishi (CRIEPI)
- Estimation of STT1b and STT1, and Blind prediction of the STT-1 tracer tests with multiple rates of mass transfer. S McKenna (DOE/Sandia)
- Blind predictions for the Task 4F (STT2) tracer migration experiment at the Äspö TRUE-1 site. A Jakob, W Heer (NAGRA/PSI)



## **B.1 Comparisons of STT2 modelling results**





## TASK NO 4F – COMPILATION OF PREDICTIVE MODELLING RESULTS OF THE STT-2 TRACER EXPERIMENTS WITHIN TRUE-1

The following is a compilation of results from a predictive modelling exercise of the STT-2 tracer experiment within the TRUE-1 project performed by nine different modelling groups. The modelling teams are presented in Table 1. The results are compiled in four groups, according to modelling approach and type of data modelled,

1. Stochastic models on mass recovery
2. Deterministic models on mass recovery
3. Stochastic models of breakthrough times
4. Deterministic models of breakthrough times

Table 1 Modelling teams and their model approach to Task 4F.

MODELLING TEAM	MODEL APPROACH	AUTHOR
ANDRA / CEA	Deterministic	Grenier & Mouche
BMW / BGR	Deterministic	Shao & Liedtke
CRIEPI	Deterministic	Tanaka et al
DOE / SANDIA	Deterministic	McKenna
JNC / Golder	Deterministic	Cladouhos et al
NAGRA / PSI	Deterministic	Jakob & Heer
POSIVA / VTT	Deterministic	Poteri
SKB / KTH-KAT	Stochastic	Moreno
SKB / TRUE	Deterministic	Cvetkovic et al
Experimental results	Results from field tracer experiments	Andersson et al

The modelling groups have predicted the breakthrough of the non-sorbing tracers; Uranine (except SKB / TRUE), tritiated water (HTO), and Br (except CRIEPI and POSIVA / VTT) and the sorbing tracers Ca, Na and Sr. All groups except ANDRA / CEA have also modelled the sorbing tracers Ba, Cs and Rb. Breakthrough times for the tracers are presented in tables and diagrams. The predictive breakthrough of the ten different tracers is shown in two different ways; as mass flux (Bq/h or mg/h) versus time (h) and as cumulative percentage versus time. The  $t_5$ ,  $t_{50}$  and  $t_{95}$  for each tracer are shown as histograms and in tables. In the tables the results are divided between the stochastic and deterministic models. In the histograms both types of models are shown in the same diagram where data from the stochastic models are taken from the 50% column.

All groups except BMBF / BGR have also modelled the tracers with a Dirac pulse. The results are presented as diagrams with cumulative percentage versus time.

## 1. STOCHASTIC MODELS OF MASS RECOVERY

Table 1 Mass recovery of Barium (Ba-131). Unit for mass recovery is (%). The detection time ( $T_{100}$ ) unit is hours.

Modelling team	$F_c$ (5%)	$F_c$ (50%)	$F_c$ (95%)	$T_{100}$ (h)
SKB / KTH - KAT	3	44	79	8000
<i>Experimental results</i>		56		1130

Table 2 Mass recovery of Barium (Ba-133). Unit for mass recovery is (%). The detection time ( $T_{100}$ ) unit is hours.

Modelling team	$F_c$ (5%)	$F_c$ (50%)	$F_c$ (95%)	$T_{100}$ (h)
SKB / KTH - KAT	7	59	86	8000
<i>Experimental results</i>		66		3078

Table 3 Mass recovery of Bromine (Br-82). Unit for mass recovery is (%). The detection time ( $T_{100}$ ) unit is hours.

Modelling team	$F_c$ (5%)	$F_c$ (50%)	$F_c$ (95%)	$T_{100}$ (h)
SKB / KTH - KAT	24	83	99	8000
<i>Experimental results</i>		85		234

Table 4 Mass recovery of Calcium (Ca-47). Unit for mass recovery is (%). The detection time ( $T_{100}$ ) unit is hours.

Modelling team	$F_c$ (5%)	$F_c$ (50%)	$F_c$ (95%)	$T_{100}$ (h)
SKB / KTH - KAT	14	70	93	8000
<i>Experimental results</i>		97		456

Table 5 Mass recovery of Caesium (Cs-134). Unit for mass recovery is (%). The detection time ( $T_{100}$ ) unit is hours.

Modelling team	$F_c$ (5%)	$F_c$ (50%)	$F_c$ (95%)	$T_{100}$ (h)
SKB / KTH - KAT	0	5	35	8000
<i>Experimental results</i>		11		3078

Table 6 Mass recovery of Tritiated water (HTO). Unit for mass recovery is (%). The detection time ( $T_{100}$ ) unit is hours.

Modelling team	$F_c$ (5%)	$F_c$ (50%)	$F_c$ (95%)	$T_{100}$ (h)
SKB / KTH - KAT	24	83	100	8000
<i>Experimental results</i>		83		640

Table 7 Mass recovery of Sodium (Na-22). Unit for mass recovery is (%). The detection time ( $T_{100}$ ) unit is hours.

Modelling team	$F_c$ (5%)	$F_c$ (50%)	$F_c$ (95%)	$T_{100}$ (h)
SKB / KTH - KAT	24	83	100	8000
<i>Experimental results</i>		83		3078

Table 8 Mass recovery of Rubidium (Rb-86). Unit for mass recovery is (%). The detection time ( $T_{100}$ ) unit is hours.

Modelling team	$F_c$ (5%)	$F_c$ (50%)	$F_c$ (95%)	$T_{100}$ (h)
SKB / KTH - KAT	0	26	65	8000
<i>Experimental results</i>		49		1322

Table 9 Mass recovery of Strontium (Sr-85). Unit for mass recovery is (%). The detection time ( $T_{100}$ ) unit is hours.

Modelling team	$F_c$ (5%)	$F_c$ (50%)	$F_c$ (95%)	$T_{100}$ (h)
SKB / KTH - KAT	23	80	97	8000
<i>Experimental results</i>		79		3078

Table 10 Mass recovery of Uranine. Unit for mass recovery is (%). The detection time ( $T_{100}$ ) unit is hours.

Modelling team	$F_c$ (5%)	$F_c$ (50%)	$F_c$ (95%)	$T_{100}$ (h)
SKB / KTH - KAT	25	83	100	8000
<i>Experimental results</i>		96		885

## 2. DETERMINISTIC MODELS OF MASS RECOVERY

Table 1 Mass recovery of Barium (Ba-131). Unit for mass recovery is (%). The detection time ( $T_{100}$ ) unit is hours.

Modelling team	$F_c$ (%)	$T_{100}$ (h)
ANDRA / CEA	-	-
BMBF / BGR	84	1130
CRIEPI	75.46	1130
DOE / SANDIA	81.8	1130
JNC / Golder	18.3	1130
NAGRA / PSI	75.4	1130
POSIVA / VTT	81	1130
SKB / TRUE	83	1130
<i>Experimental results</i>	56	1130

Table 2 Mass recovery of Barium (Ba-133). Unit for mass recovery is (%). The detection time ( $T_{100}$ ) unit is hours.

Modelling team	$F_c$ (%)	$T_{100}$ (h)
ANDRA / CEA	-	-
BMBF / BGR	100	3078
CRIEPI	85.42	3078
DOE / SANDIA	94.1	3078
JNC / Golder	76.1	3078
NAGRA / PSI	93.0	3078
POSIVA / VTT	89	3078
SKB / TRUE	90	3078
<i>Experimental results</i>	66	3078

Table 3 Mass recovery of Bromine (Br-82). Unit for mass recovery is (%). The detection time ( $T_{100}$ ) unit is hours.

Modelling team	$F_c$ (%)	$T_{100}$ (h)
ANDRA / CEA	79	234
BMBF / BGR	46	234
CRIEPI	-	-
JNC / Golder	57.1	234
NAGRA / PSI	95.7	234
DOE / SANDIA	92.5	234
POSIVA / VTT	-	-
SKB / TRUE	95	234
<i>Experimental results</i>	85	234

Table 4 Mass recovery of Calcium (Ca-47). Unit for mass recovery is (%). The detection time ( $T_{100}$ ) unit is hours.

Modelling team	$F_c$ (%)	$T_{100}$ (h)
ANDRA / CEA	56	456
BMBF / BGR	49.7	458
CRIEPI	90.14	458
JNC / Golder	50.7	458
NAGRA / PSI	92.4	458
DOE / SANDIA	100	458
POSIVA / VTT	91	458
SKB / TRUE	96	458
<i>Experimental results</i>	97	456

Table 5 Mass recovery of Caesium (Cs-134). Unit for mass recovery is (%). The detection time ( $T_{100}$ ) unit is hours.

Modelling team	$F_c$ (%)	$T_{100}$ (h)
ANDRA / CEA	-	-
BMBF / BGR	5.6	3078
CRIEPI	24.31	3078
JNC / Golder	16.8	3078
NAGRA / PSI	15.5	3078
DOE / SANDIA	33.7	3078
POSIVA / VTT	66	3078
SKB / TRUE	15	3078
<i>Experimental results</i>	11	3078

Table 6 Mass recovery of Tritiated water (HTO). Unit for mass recovery is (%). The detection time ( $T_{100}$ ) unit is hours.

Modelling team	$F_c$ (%)	$T_{100}$ (h)
ANDRA / CEA	100	640
BMBF / BGR	99	641
CRIEPI	99.81	641
JNC / Golder	100.0	641
NAGRA / PSI	100.0	641
DOE / SANDIA	97.8	641
POSIVA / VTT	99	641
SKB / TRUE	99	641
<i>Experimental results</i>	83	640

Table 7 Mass recovery of Sodium (Na-22). Unit for mass recovery is (%). The detection time ( $T_{100}$ ) unit is hours.

Modelling team	$F_c$ (%)	$T_{100}$ (h)
ANDRA / CEA	100	3078
BMBF / BGR	100	3078
CRIEPI	97.61	3078
JNC / Golder	100.0	3078
NAGRA / PSI	100.0	3078
DOE / SANDIA	99.4	3078
POSIVA / VTT	97	3078
SKB / TRUE	100	3078
<i>Experimental results</i>	83	3078

Table 8 Mass recovery of Rubidium (Rb-86). Unit for mass recovery is (%). The detection time ( $T_{100}$ ) unit is hours.

Modelling team	$F_c$ (%)	$T_{100}$ (h)
ANDRA / CEA	-	-
BMBF / BGR	14.4	1322
CRIEPI	60.87	1322
JNC / Golder	8.3	1322
NAGRA / PSI	71.0	1322
DOE / SANDIA	70.0	1322
POSIVA / VTT	70	1322
SKB / TRUE	67	1322
<i>Experimental results</i>	49	1322

Table 9 Mass recovery of Strontium (Sr-85). Unit for mass recovery is (%). The detection time ( $T_{100}$ ) unit is hours.

Modelling team	$F_c$ (%)	$T_{100}$ (h)
ANDRA / CEA	96	3078
BMBF / BGR	93	3078
CRIEPI	95.7	3078
JNC / Golder	89.6	3078
NAGRA / PSI	100.0	3078
DOE / SANDIA	98.1	3078
POSIVA / VTT	95	3078
SKB / TRUE	100	3078
<i>Experimental results</i>	79	3078

Table 10 Mass recovery of Uranine. Unit for mass recovery is (%). The detection time ( $T_{100}$ ) unit is hours.

Modelling team	$F_c$ (%)	$T_{100}$ (h)
ANDRA / CEA	100	885
BMBF / BGR	100	886
CRIEPI	99.97	886
JNC / Golder	100.0	886
NAGRA / PSI	100.0	886
DOE / SANDIA	99.4	886
POSIVA / VTT	99	886
SKB / TRUE	-	-
<i>Experimental results</i>	96	885

### 3. STOCHASTIC MODELS OF BREAKTHROUGH TIMES

Table 1 Breakthrough times for Barium (Ba-131) in the stochastic model. Unit for measured input functions is hours. The experimental results are based on injected mass at 592 h.

Modelling team	t5 (5%)	t5 (50%)	t5 (95%)	t50 (5%)	t50 (50%)	t50 (95%)	t95 (5%)	t95 (50%)	t95 (95%)
SKB / KTH - KAT	25.0	111.4	-	250.4	1681.7	-	-	-	-
<i>Experimental results</i>		84.3			916			-	

Table 2 Breakthrough times for Barium (Ba-133) in the stochastic model. Unit for measured input functions is hours. The experimental results are based on injected mass at 856 h.

Modelling team	t5 (5%)	t5 (50%)	t5 (95%)	t50 (5%)	t50 (50%)	t50 (95%)	t95 (5%)	t95 (50%)	t95 (95%)
SKB / KTH - KAT	24.4	112.4	3068.3	251.9	1811.7	-	-	-	-
<i>Experimental results</i>		82.3			949			-	

Table 3 Breakthrough times for Bromine (Br-82) in the stochastic model. Unit for measured input functions is hours. The experimental results are based on injected mass at 212 h.

Modelling team	t5 (5%)	t5 (50%)	t5 (95%)	t50 (5%)	t50 (50%)	t50 (95%)	t95 (5%)	t95 (50%)	t95 (95%)
SKB / KTH - KAT	4.7	8.7	38.2	39.3	58.9	-	178.2	-	-
<i>Experimental results</i>		12.3			86			-	

Table 4 Breakthrough times for Calcium (Ca-47) in the stochastic model. Unit for measured input functions is hours. The experimental results are based on injected mass at 242 h.

Modelling team	t5 (5%)	t5 (50%)	t5 (95%)	t50 (5%)	t50 (50%)	t50 (95%)	t95 (5%)	t95 (50%)	t95 (95%)
SKB / KTH - KAT	6.2	14.8	177.8	62.1	142.9	-	959.3	-	-
<i>Experimental results</i>		25.8			145		433		



Table 5 Breakthrough times for Caesium (Cs-134) in the stochastic model. Unit for measured input functions is hours. The experimental results are based on injected mass at 1848 h.

Modelling team	t5 (5%)	t5 (50%)	t5 (95%)	t50 (5%)	t50 (50%)	t50 (95%)	t95 (5%)	t95 (50%)	t95 (95%)
SKB / KTH - KAT	728.3	3948.6	-	-	-	-	-	-	-
<i>Experimental results</i>		1528							

Table 6 Breakthrough times for Tritiated water (HTO) in the stochastic model. Unit for measured input functions is hours. The experimental results are based on injected mass at 578 h.

Modelling team	t5 (5%)	t5 (50%)	t5 (95%)	t50 (5%)	t50 (50%)	t50 (95%)	t95 (5%)	t95 (50%)	t95 (95%)
SKB / KTH - KAT	4.7	8.8	40.5	43.0	62.2	377.5	-	-	-
<i>Experimental results</i>		13.5			91				

Table 7 Breakthrough times for Sodium (Na-22) in the stochastic model. Unit for measured input functions is hours. The experimental results are based on injected mass at 664 h.

Modelling team	t5 (5%)	t5 (50%)	t5 (95%)	t50 (5%)	t50 (50%)	t50 (95%)	t95 (5%)	t95 (50%)	t95 (95%)
SKB / KTH - KAT	5.3	9.7	43.3	43.4	62.5	-	265.1	-	-
<i>Experimental results</i>		18.8			120				

Table 8 Breakthrough times for Rubidium (Rb-86) in the stochastic model. Unit for measured input functions is hours. The experimental results are based on injected mass at 458 h.

Modelling team	t5 (5%)	t5 (50%)	t5 (95%)	t50 (5%)	t50 (50%)	t50 (95%)	t95 (5%)	t95 (50%)	t95 (95%)
SKB / KTH - KAT	63.2	310.3	-	555.3	-	-	-	-	-
<i>Experimental results</i>		157.6							

Table 9 Breakthrough times for Strontium (Sr-85) in the stochastic model. Unit for measured input functions is hours. The experimental results are based on injected mass at 904 h.

Modelling team	t5 (5%)	t5 (50%)	t5 (95%)	t50 (5%)	t50 (50%)	t50 (95%)	t95 (5%)	t95 (50%)	t95 (95%)
SKB / KTH - KAT	6.2	15.1	168.7	64.9	148.0	-	968.6	-	-
<i>Experimental results</i>		30.6			190				-

Table 10 Breakthrough times for Uranine in the stochastic model. Unit for measured input functions is hours. The experimental results are based on injected mass at 828 h.

Modelling team	t5 (5%)	t5 (50%)	t5 (95%)	t50 (5%)	t50 (50%)	t50 (95%)	t95 (5%)	t95 (50%)	t95 (95%)
SKB / KTH - KAT	5.0	9.2	42.5	47.5	67.0	-	244.1	-	-
<i>Experimental results</i>		11.2			79			805	

#### 4. DETERMINISTIC MODELS OF BREAKTHROUGH TIMES

Table 1 Breakthrough times for Barium (Ba-131) in the deterministic models. Unit for measured input functions is hours. The experimental results are based on injected mass at 592 h.

Modelling team	t <sub>5%</sub>	t <sub>50%</sub>	t <sub>95%</sub>
ANDRA / CEA	-	-	-
BMBF / BGR	50	500	-
CRIEPI	47.20	368.93	-
DOE / SANDIA	50.37	320.96	3467.5
JNC / Golder	162.7	1130.7	-
NAGRA / PSI	47	378	3670
POSIVA / VTT	60	312	-
SKB / TRUE	57.3	279.2	6389.4
<i>Experimental results</i>	84.3	916	-

Table 2 Breakthrough times for Barium (Ba-133) in the deterministic models. Unit for measured input functions is hours. The experimental results are based on injected mass at 856 h.

Modelling team	t <sub>5%</sub>	t <sub>50%</sub>	t <sub>95%</sub>
ANDRA / CEA	-	-	-
BMBF / BGR	50	530	1990
CRIEPI	46.03	366.43	-
DOE / SANDIA	49.74	326.97	3466.3
JNC / Golder	180.1	1106.6	-
NAGRA / PSI	46	387	3680
POSIVA / VTT	58	318	-
SKB / TRUE	56.8	283.1	6853.1
<i>Experimental results</i>	82.3	949	-

Table 3 Breakthrough times for Bromine (Br-82) in the deterministic models. Unit for measured input functions is hours. The experimental results are based on injected mass at 212 h.

Modelling team	t <sub>5%</sub>	t <sub>50%</sub>	t <sub>95%</sub>
ANDRA / CEA	10	61	-
BMBF / BGR	17	235	-
CRIEPI	-	-	-
DOE / SANDIA	9.83	67.4	304.1
JNC / Golder	9.4	135.3	-
NAGRA / PSI	8.2	81	227
POSIVA / VTT	-	-	-
SKB / TRUE	8.3	52.4	231.3
<i>Experimental results</i>	12.3	86	-

Table 4 Breakthrough times for Calcium (Ca-47) in the deterministic models. Unit for measured input functions is hours. The experimental results are based on injected mass at 242 h.

Modelling team	t <sub>5%</sub>	t <sub>50%</sub>	t <sub>95%</sub>
ANDRA / CEA	60	223	-
BMBF / BGR	12.5	115	-
CRIEPI	13.57	91.18	458.00
DOE / SANDIA	23.56	84.95	223.2
JNC / Golder	18.7	414.5	-
NAGRA / PSI	13	115	545
POSIVA / VTT	13	86	-
SKB / TRUE	14.6	67.8	348.9
<i>Experimental results</i>	25.8	145	433

Table 5 Breakthrough times for Caesium (Cs-134) in the deterministic models. Unit for measured input functions is hours. The experimental results are based on injected mass at 1848 h.

Modelling team	t <sub>5%</sub>	t <sub>50%</sub>	t <sub>95%</sub>
ANDRA / CEA	-	-	-
BMBF / BGR	840	3450	-
CRIEPI	849.01	-	-
DOE / SANDIA	876.5	4354.8	11927.4
JNC / Golder	1233.4	-	-
NAGRA / PSI	1150	-	-
POSIVA / VTT	624	2176	-
SKB / TRUE	1556.8	14304.3	459294.3
<i>Experimental results</i>	1528	-	-

Table 6 Breakthrough times for Tritiated water (HTO) in the deterministic models. Unit for measured input functions is hours. The experimental results are based on injected mass at 578 h.

Modelling team	t <sub>5%</sub>	t <sub>50%</sub>	t <sub>95%</sub>
ANDRA / CEA	10.5	49	211
BMBF / BGR	13	140	440
CRIEPI	7.87	53.50	230.98
DOE / SANDIA	9.25	71.43	373.9
JNC / Golder	11.3	61.3	229.5
NAGRA / PSI	7.1	80	280
POSIVA / VTT	5.6	48	254
SKB / TRUE	8.5	57.4	295.1
<i>Experimental results</i>	13.5	91	-

Table 7 Breakthrough times for Sodium (Na-22) in the deterministic models. Unit for measured input functions is hours. The experimental results are based on injected mass at 664 h.

Modelling team	t <sub>5%</sub>	t <sub>50%</sub>	t <sub>95%</sub>
ANDRA / CEA	25	78	263
BMBF / BGR	14	160	1590
CRIEPI	10.46	78.36	859.20
DOE / SANDIA	14.22	94.54	577.6
JNC / Golder	16.3	105.3	650.0
NAGRA / PSI	10	98	364
POSIVA / VTT	11	87	1400
SKB / TRUE	11.3	66.2	374.0
<i>Experimental results</i>	18.8	120	-

Table 8 Breakthrough times for Rubidium (Rb-86) in the deterministic models. Unit for measured input functions is hours. The experimental results are based on injected mass at 458h.

Modelling team	t <sub>5%</sub>	t <sub>50%</sub>	t <sub>95%</sub>
ANDRA / CEA	-	-	-
BMBF / BGR	243	590	-
CRIEPI	88.23	746.96	-
DOE / SANDIA	150.0	864.5	2670.9
JNC / Golder	533.5	-	-
NAGRA / PSI	94	719	3370
POSIVA / VTT	125	554	-
SKB / TRUE	118.4	660.2	8715.7
<i>Experimental results</i>	157.6	-	-

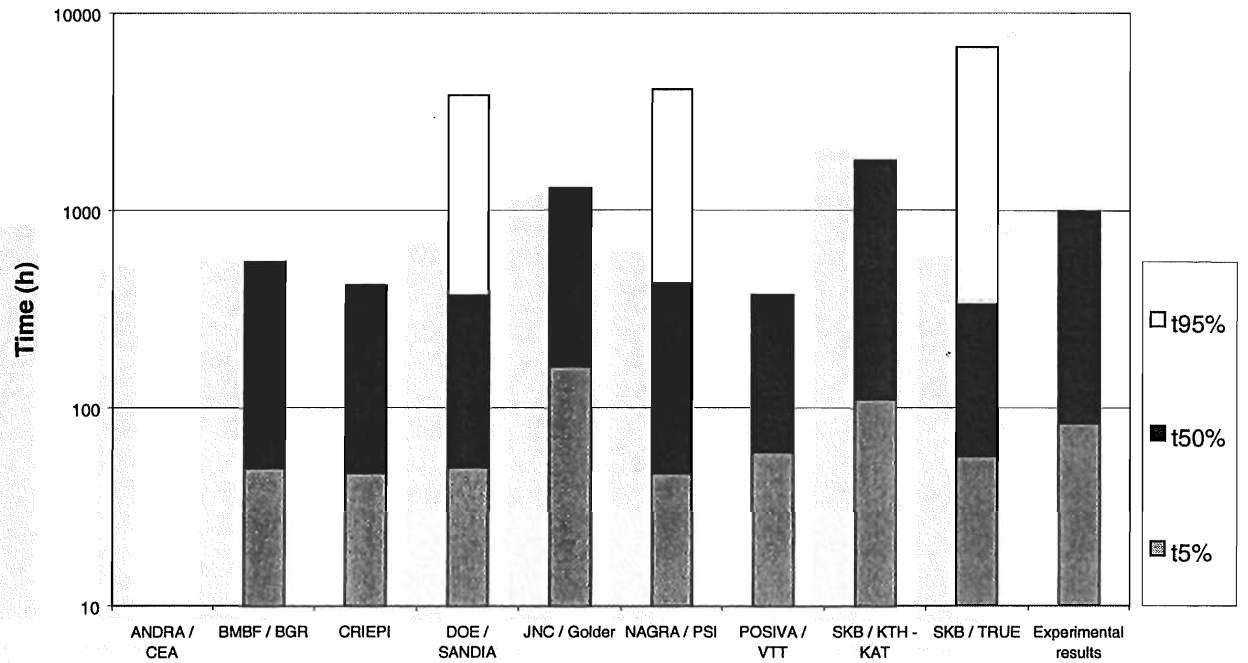
Table 9 Breakthrough times for Strontium (Sr-85) in the deterministic models. Unit for measured input functions is hours. The experimental results are based on injected mass at 904 h.

Modelling team	t <sub>5%</sub>	t <sub>50%</sub>	t <sub>95%</sub>
ANDRA / CEA	55	142	902
BMBF / BGR	16	240	-
CRIEPI	14.51	106.47	2334.41
DOE / SANDIA	19.89	128.2	1217.7
JNC / Golder	22.7	170.6	-
NAGRA / PSI	15	117	378
POSIVA / VTT	16	113	2932
SKB / TRUE	16.8	79.0	446.8
<i>Experimental results</i>	30.6	190	-

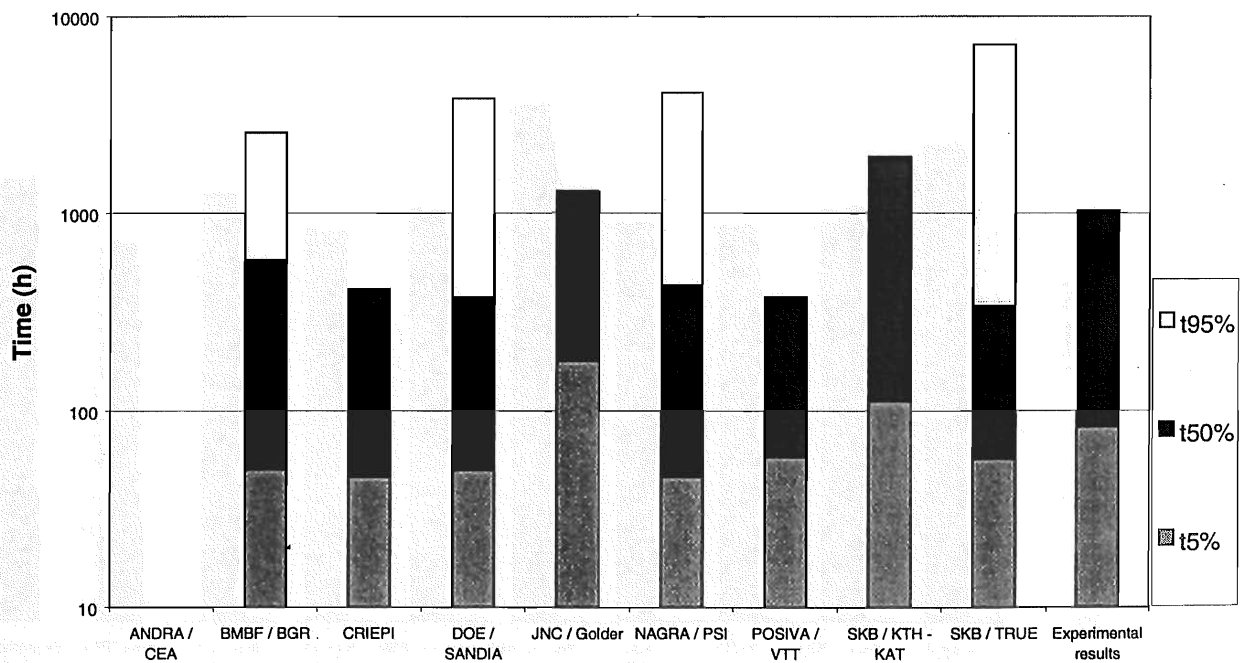
Table 10 Breakthrough times for Uranine in the deterministic models. Unit for measured input functions is hours. The experimental results are based on injected mass at 828 h.

Modelling team	t <sub>5%</sub>	t <sub>50%</sub>	t <sub>95%</sub>
ANDRA / CEA	11	54	227
BMBF / BGR	13.8	150	460
CRIEPI	8.01	55.12	226.96
DOE / SANDIA	8.48	62.68	293.0
JNC / Golder	9.7	65.3	247.9
NAGRA / PSI	6.7	78	320
POSIVA / VTT	5.7	53	276
SKB / TRUE	-	-	-
<i>Experimental results</i>	<i>11.2</i>	<i>79</i>	<i>805</i>

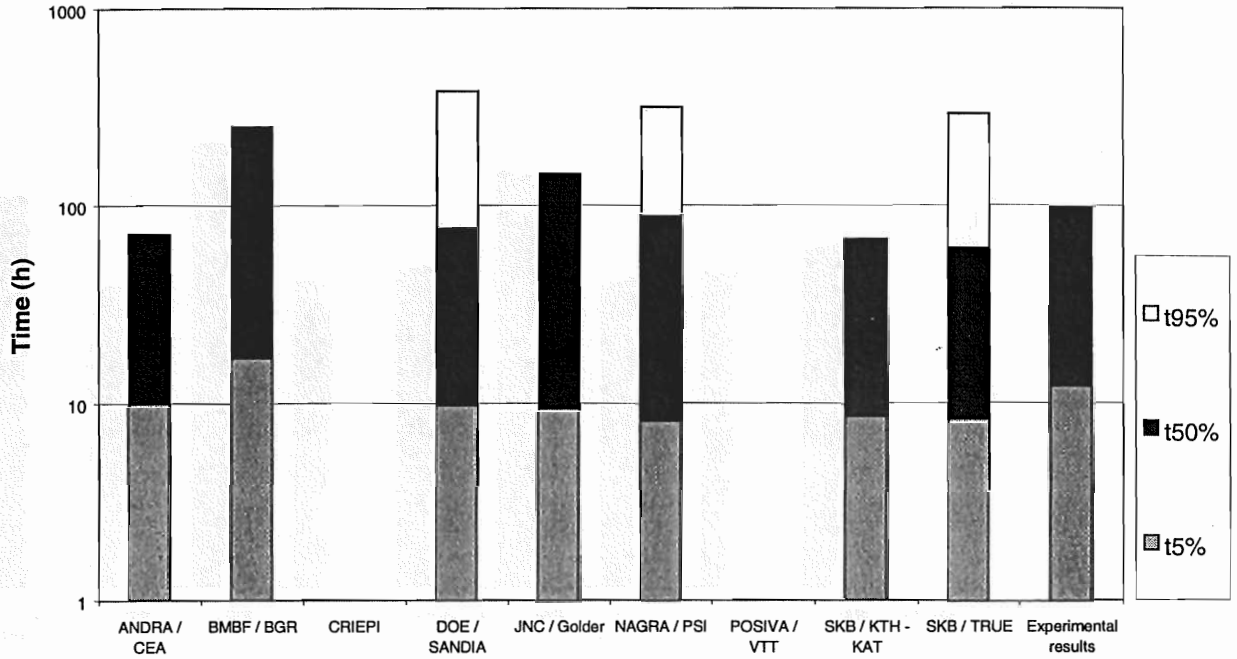
**TRUE-1 STT-2 Breakthrough Times for Barium (Ba-131)**



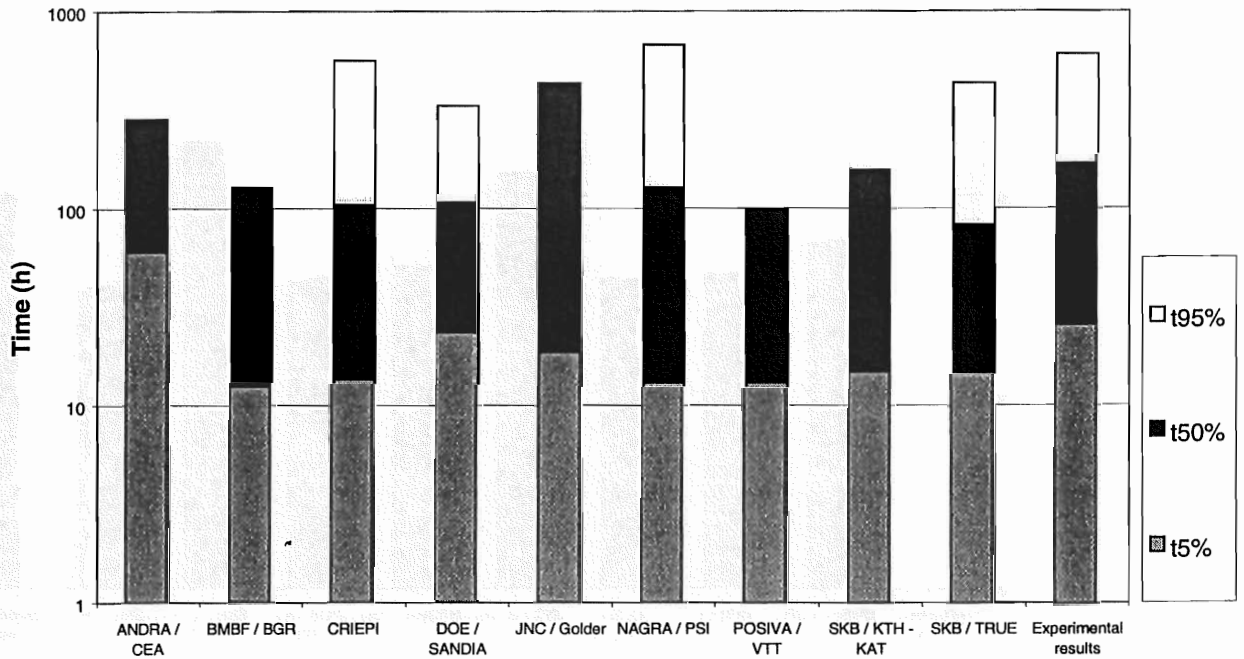
**TRUE-1 STT-2 Breakthrough Times for Barium (Ba-133)**



**TRUE-1 STT-2 Breakthrough Times for Bromine (Br-82)**

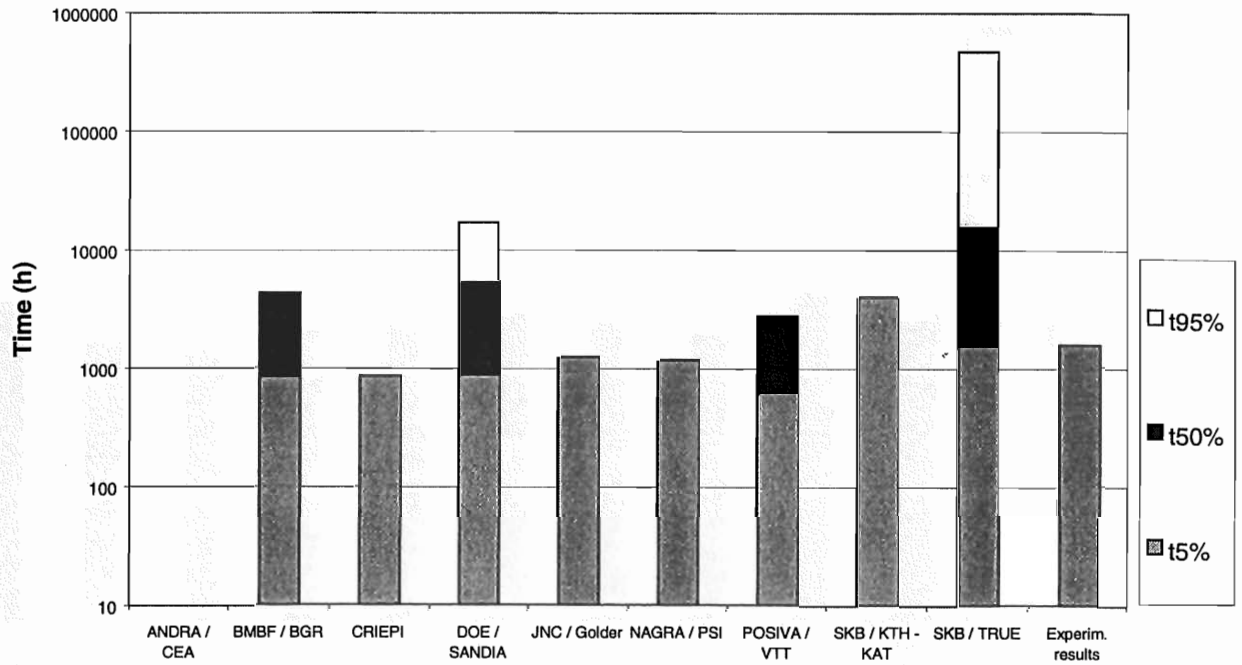


**TRUE-1 STT-2 Breakthrough Times for Calcium (Ca-47)**

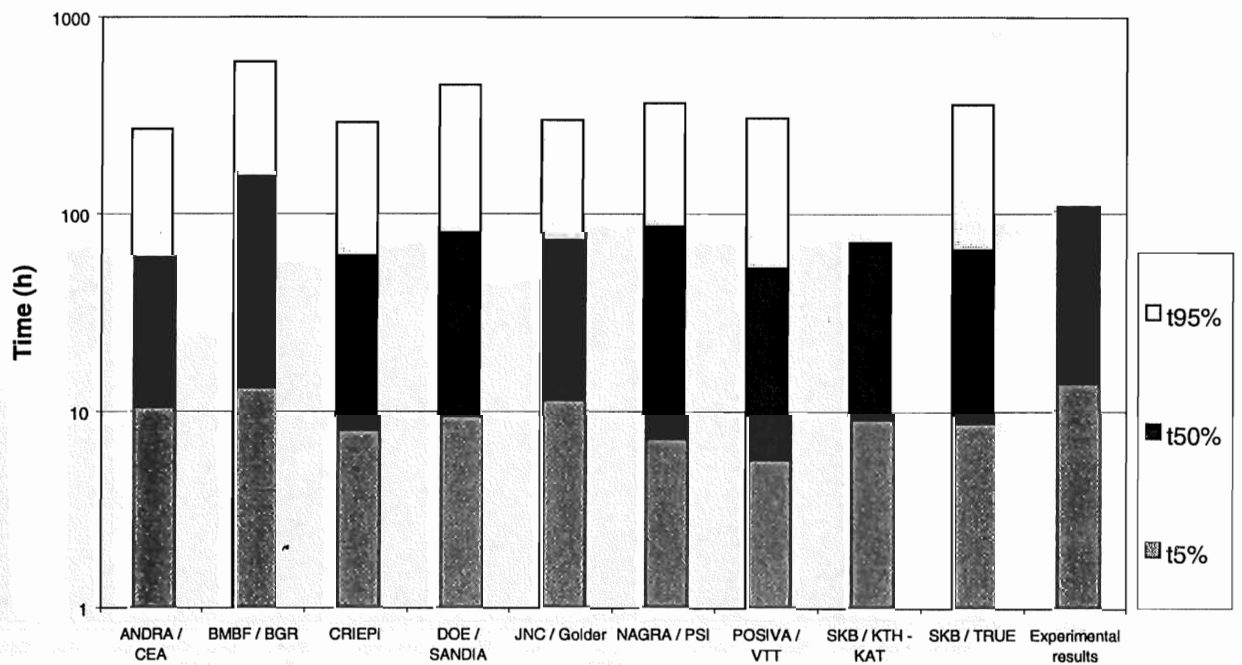




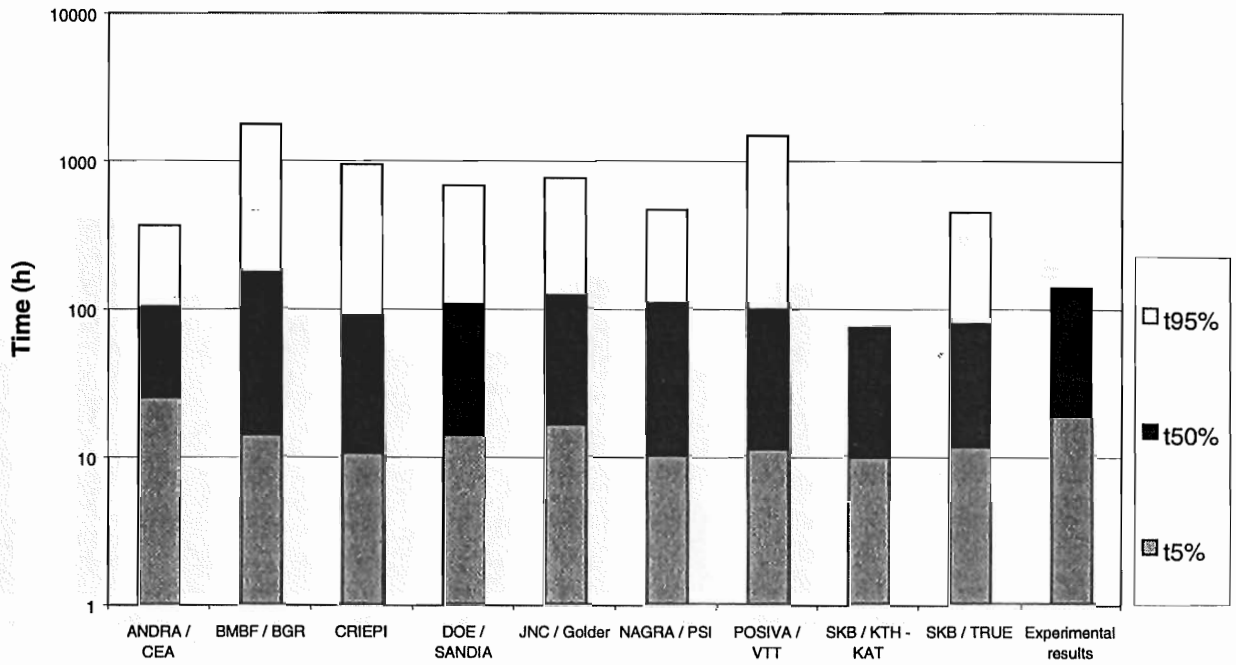
**TRUE-1 STT-2 Breakthrough Times for Caesium (Cs-134)**



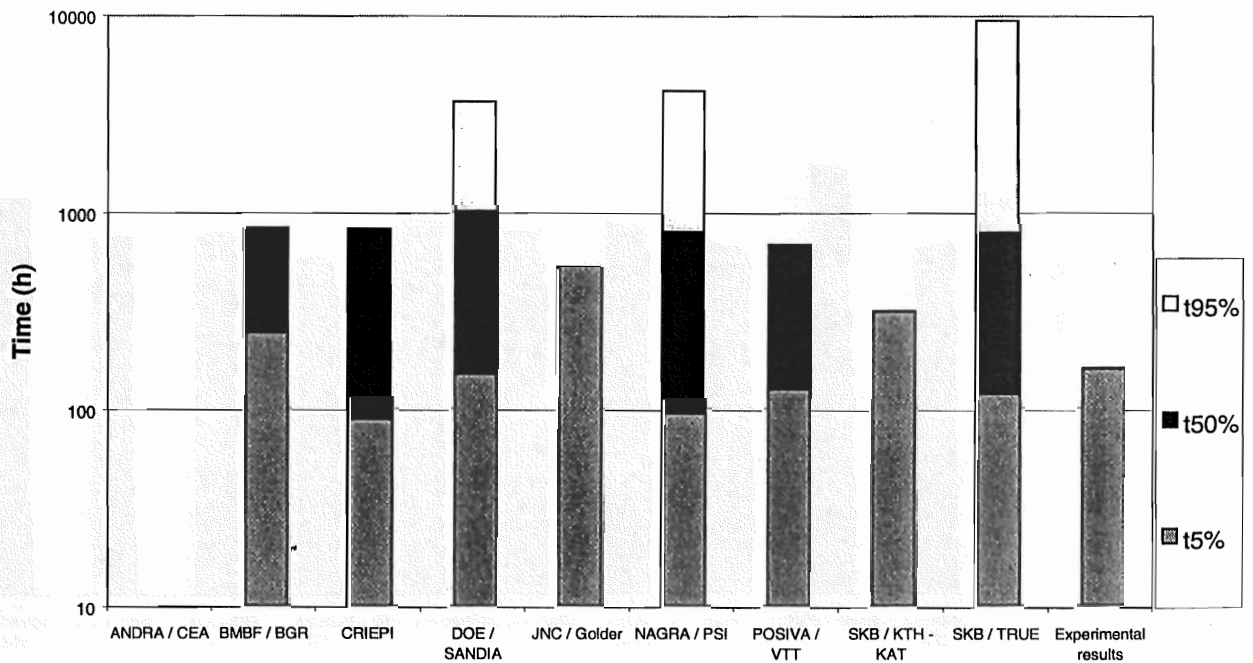
**TRUE-1 STT-2 Breakthrough Times for Tritiated Water (HTO)**



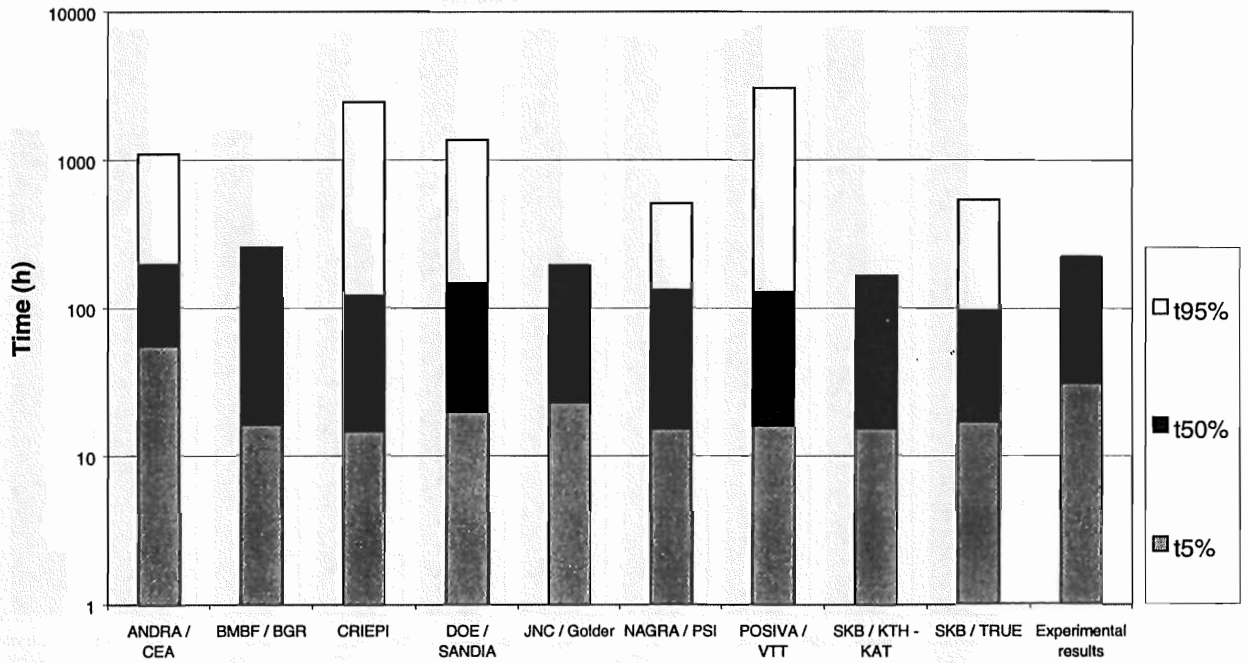
**TRUE-1 STT-2 Breakthrough Times for Sodium (Na-22)**



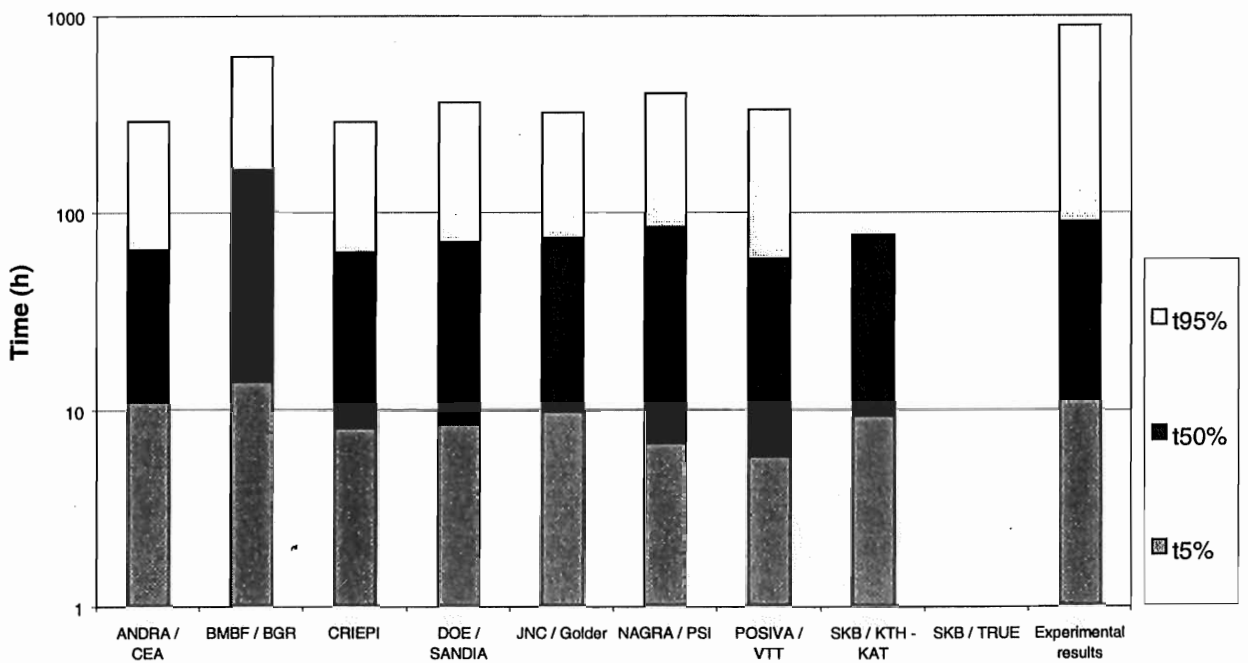
**TRUE-1 STT-1b Breakthrough Times for Rubidium (Rb-86)**



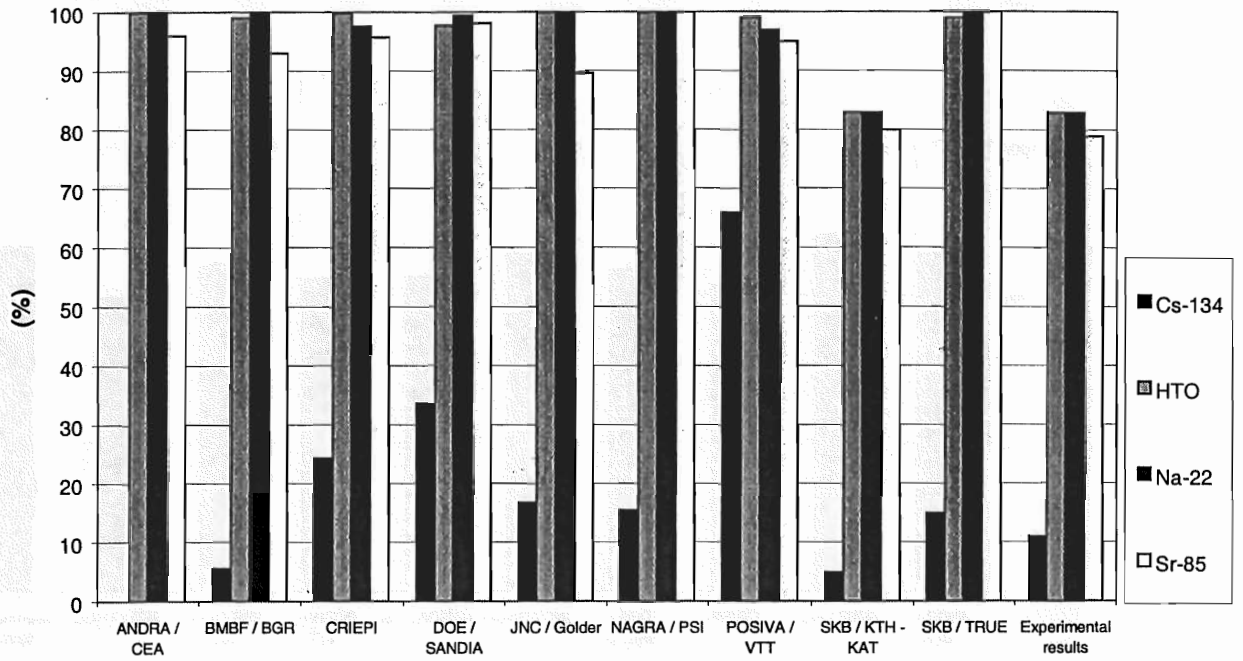
**TRUE-1 STT-2 Breakthrough Times for Strontium (Sr-85)**



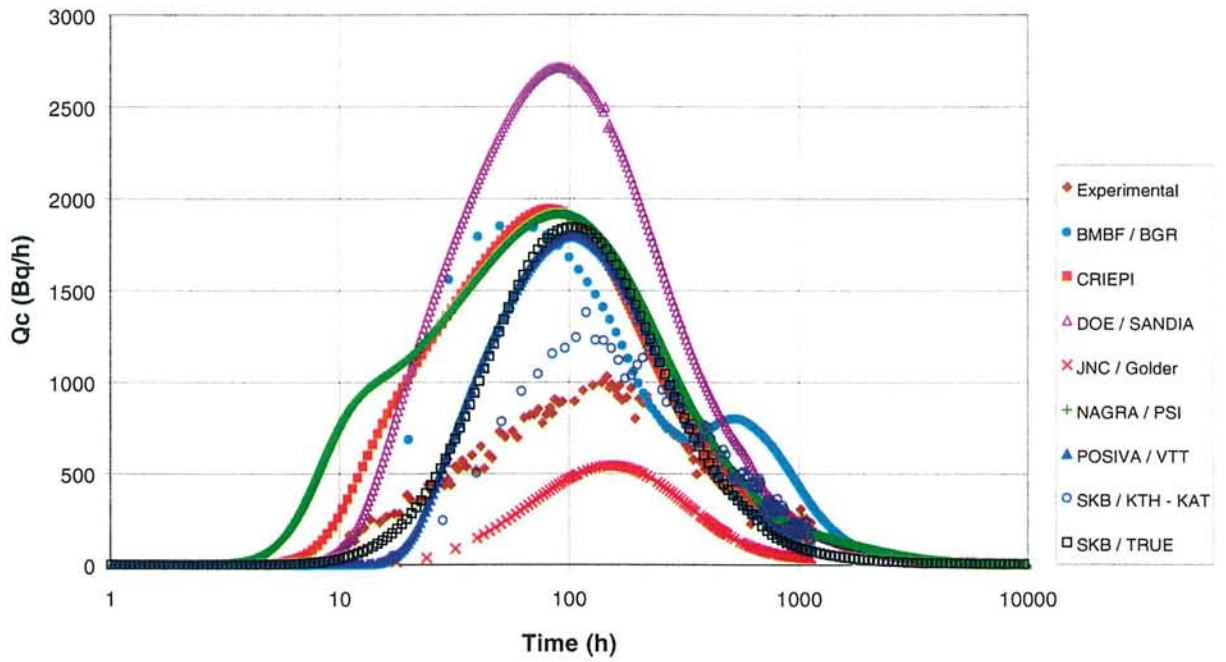
**TRUE-1 STT-2 Breakthrough Times for Uranine**



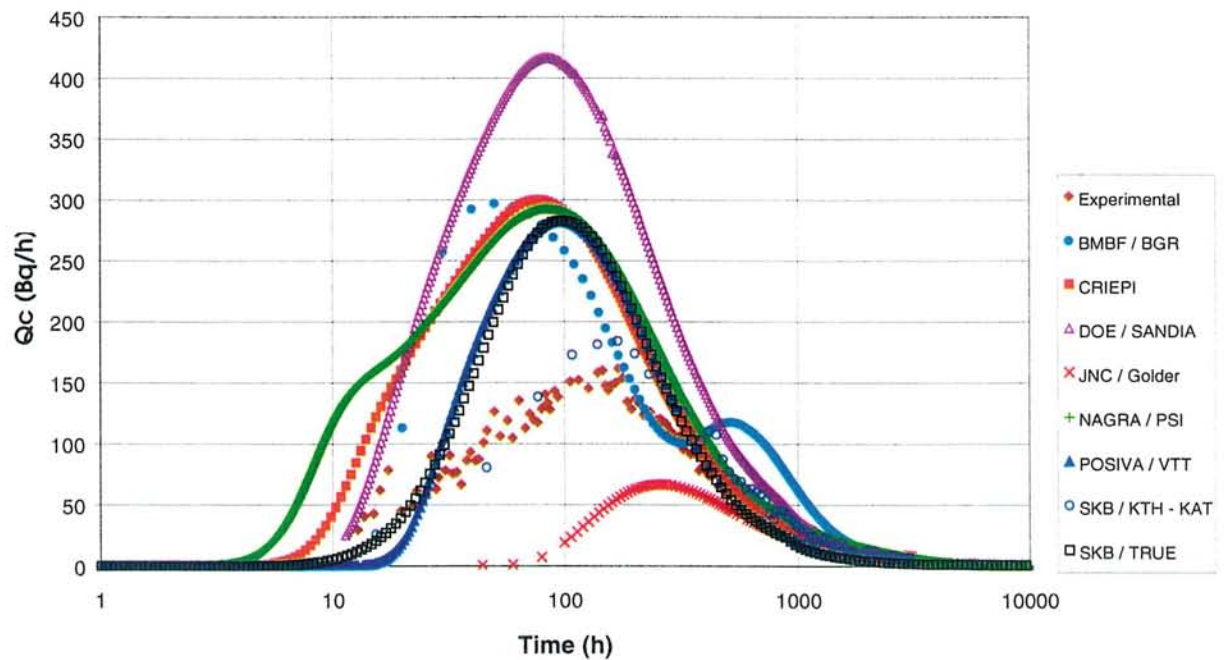
TRUE-1 STT-2 Mass Recovery  
(F50%)



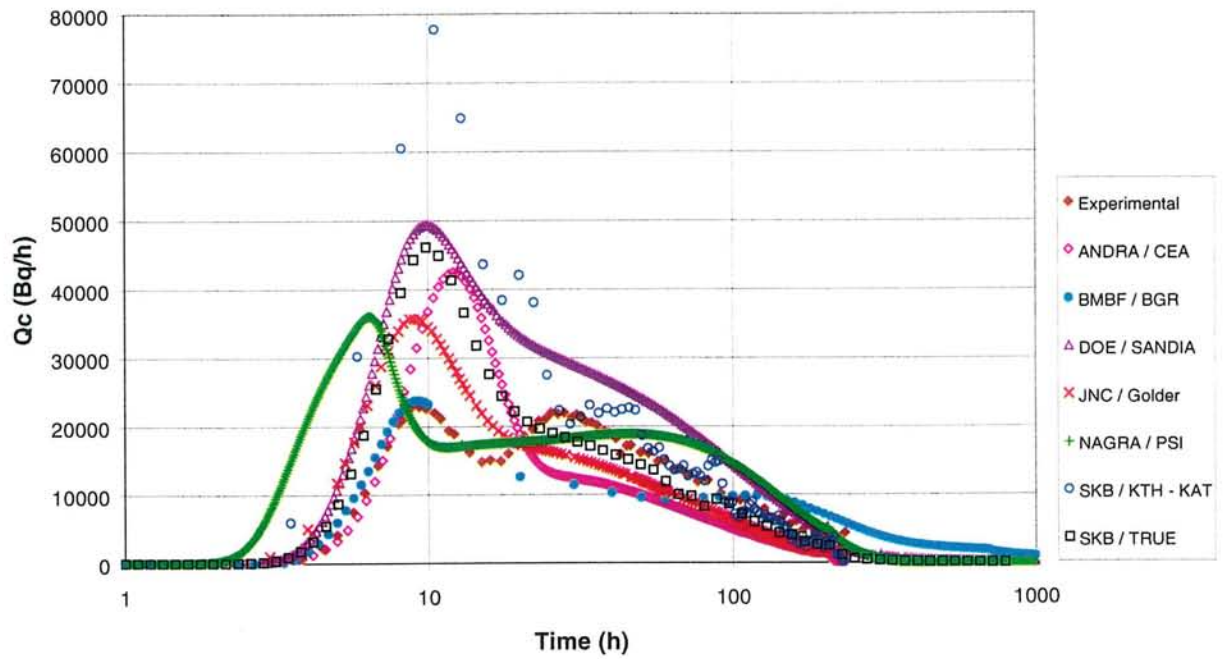
TRUE-1 STT-2 Breakthrough Curves for Ba-131



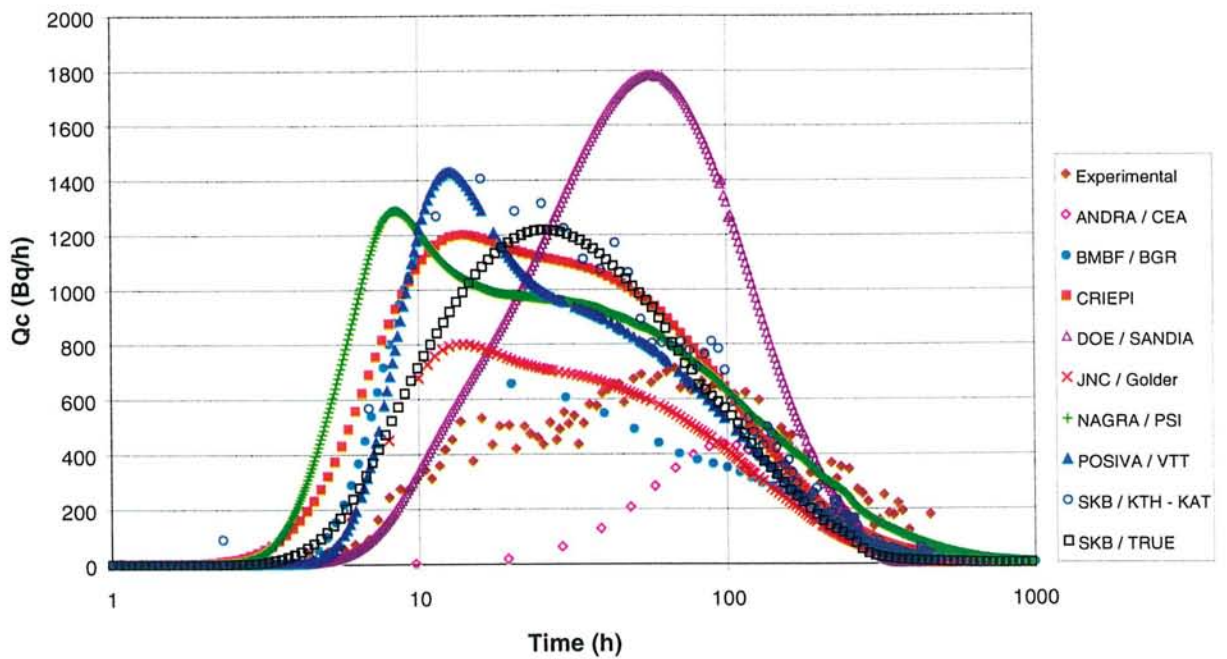
TRUE-1 STT-2 Breakthrough Curves for Ba-133



TRUE-1 STT-2 Breakthrough Curves for Br-82

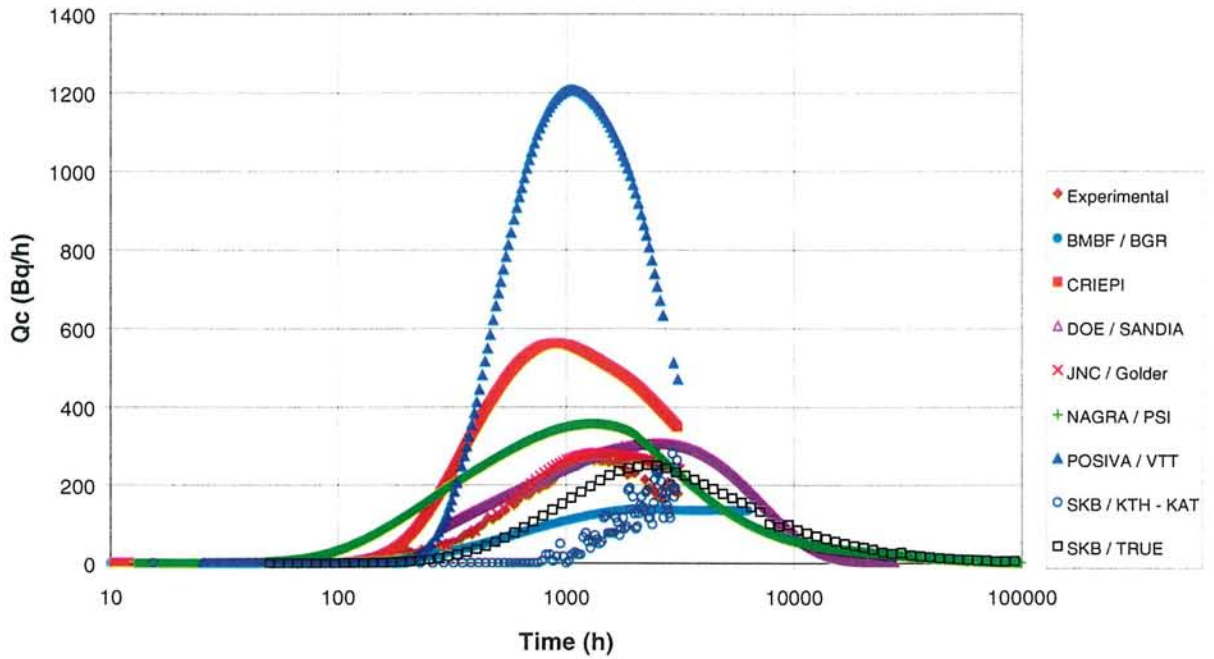


TRUE-1 STT-2 Breakthrough Curves for Ca-47

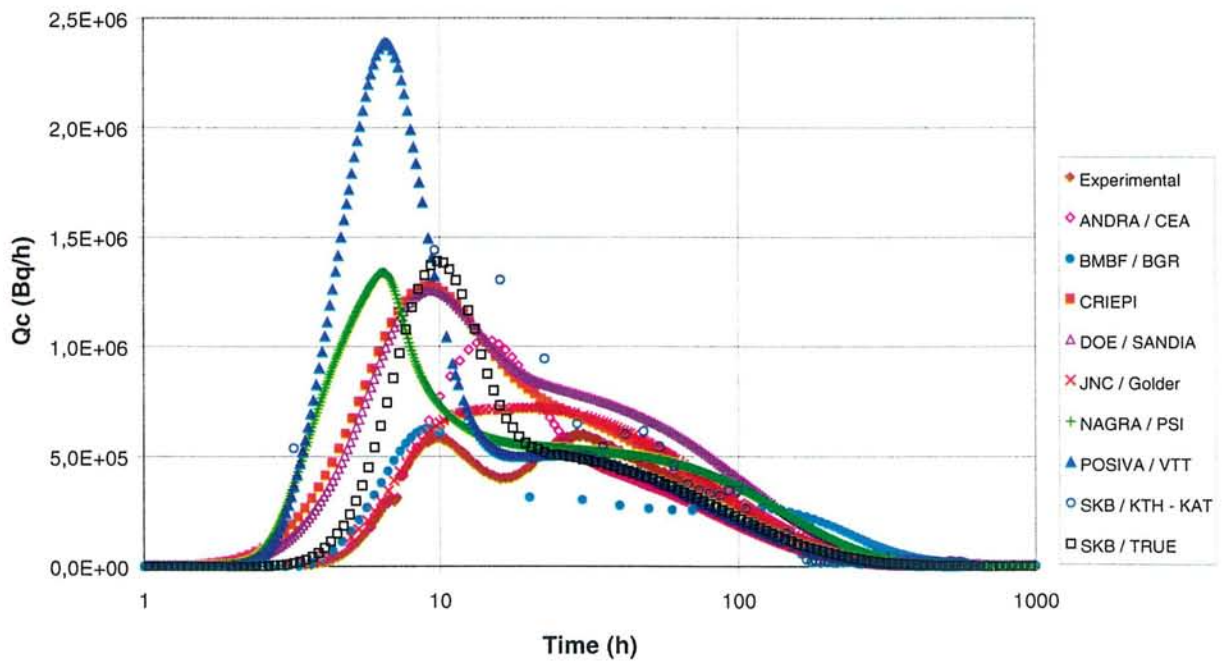




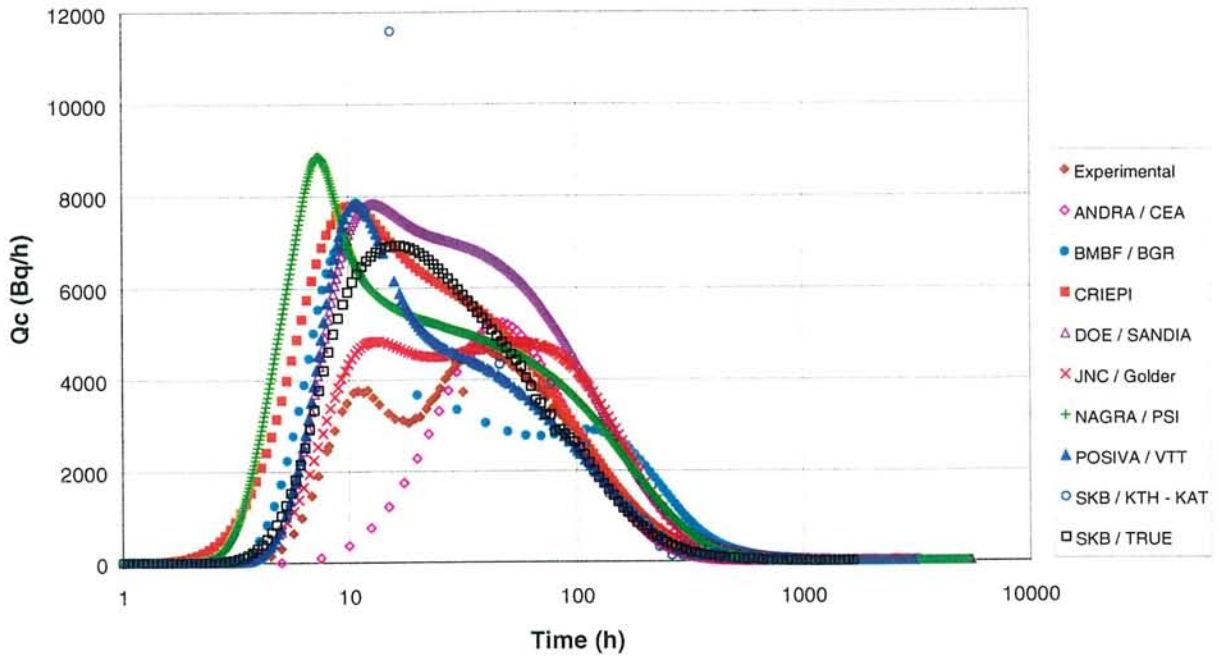
### TRUE-1 STT-2 Breakthrough Curves for Cs-134



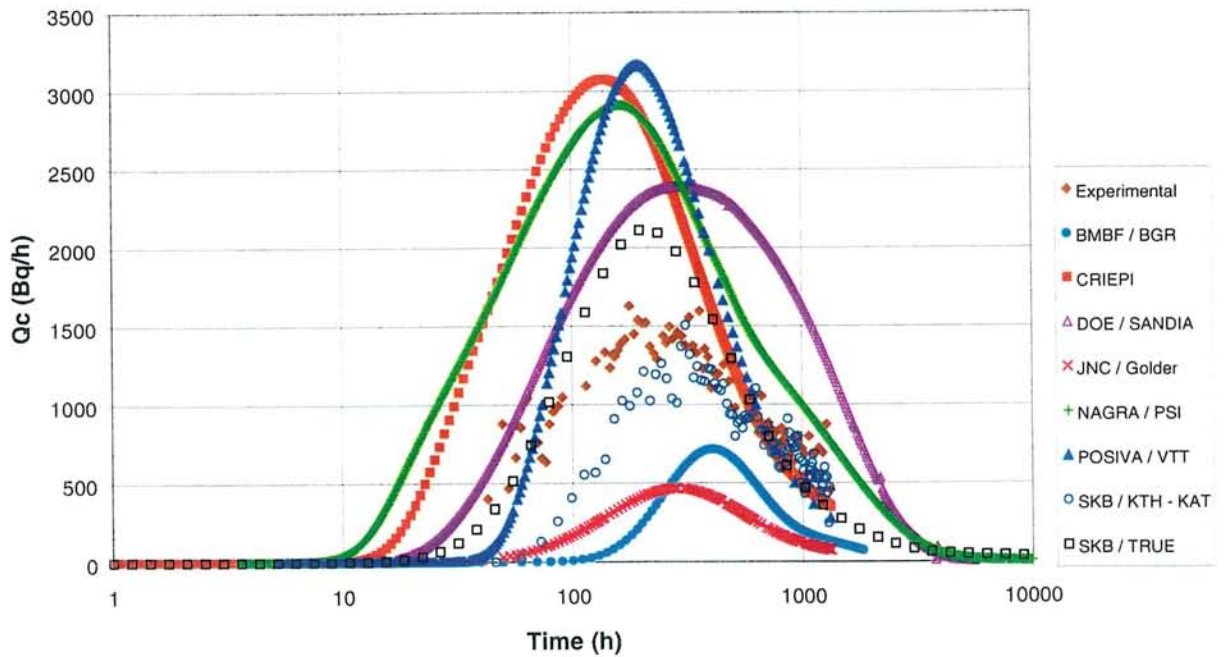
### TRUE-1 STT-2 Breakthrough Curves for Tritiated Water



**TRUE-1 STT-2 Breakthrough Curves for Na-22**

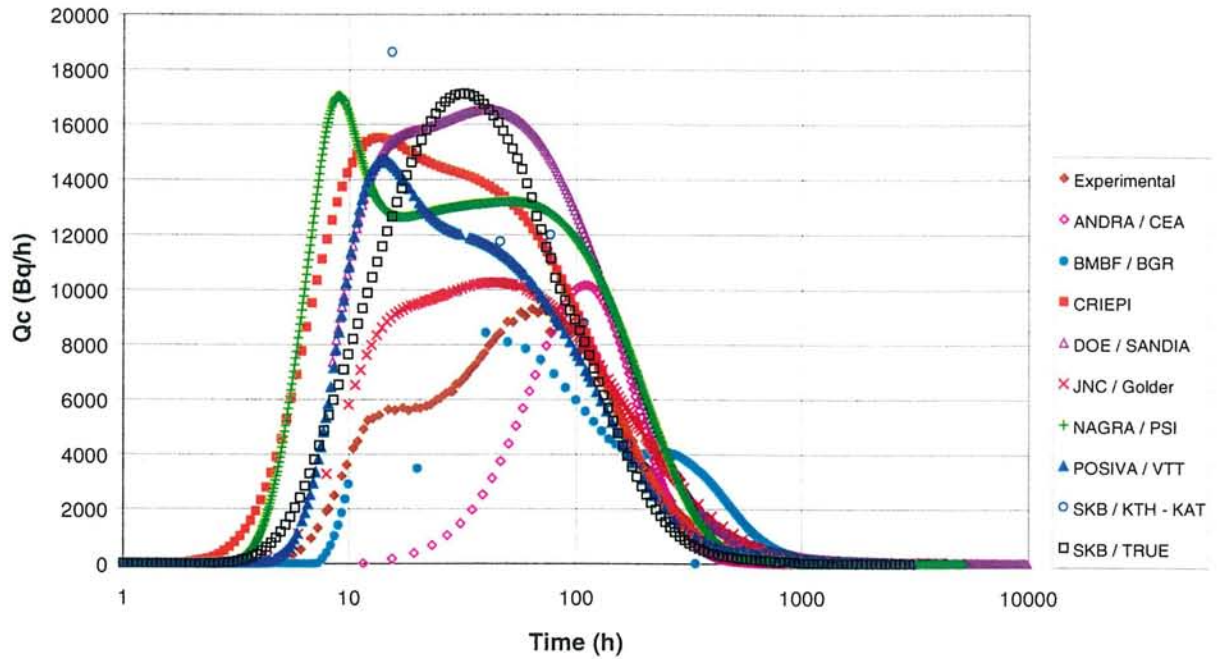


**TRUE-1 STT-2 Breakthrough Curves for Rb-86**

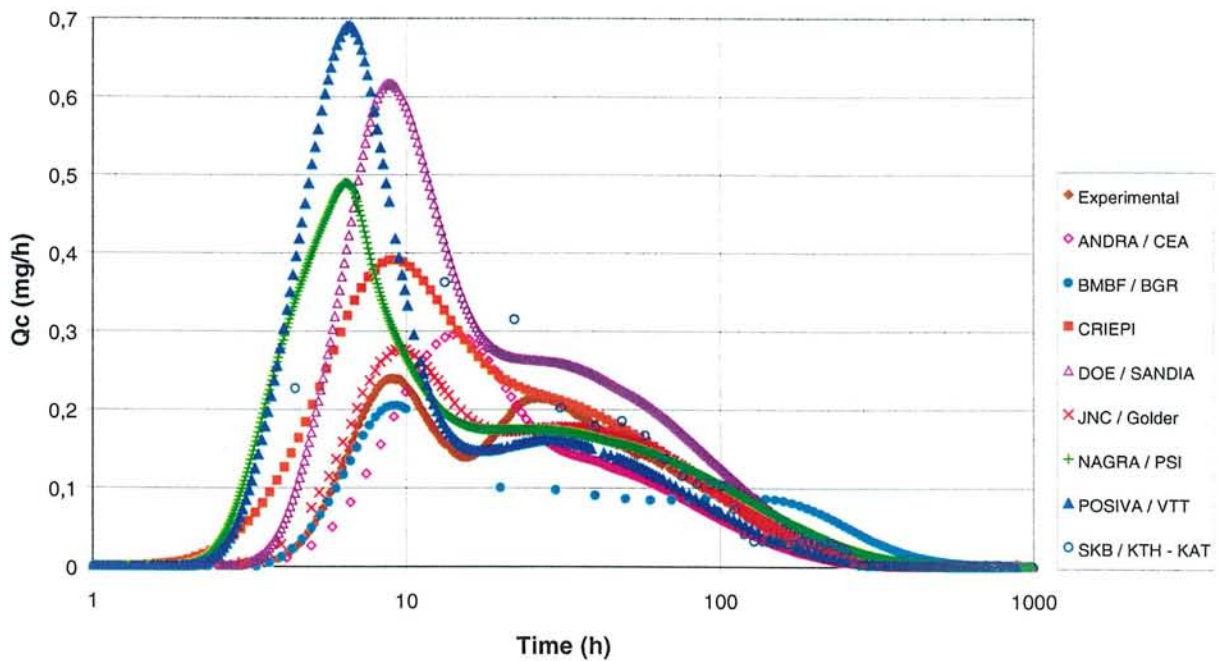




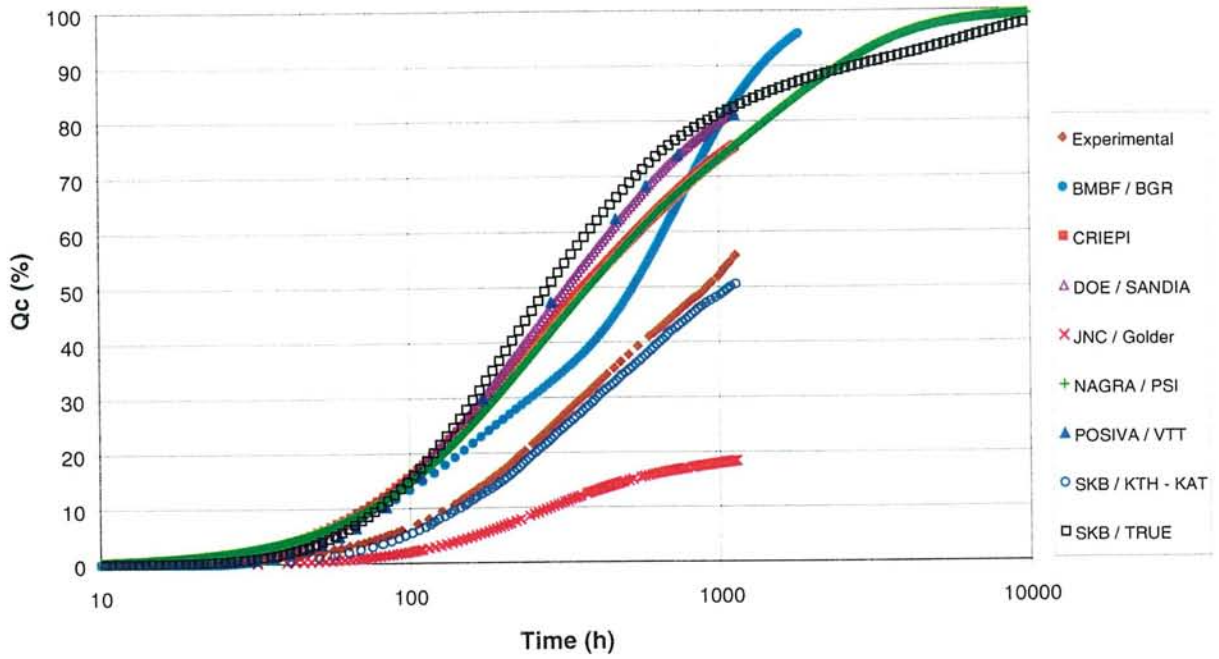
### TRUE-1 STT-2 Breakthrough Curves for Sr-85



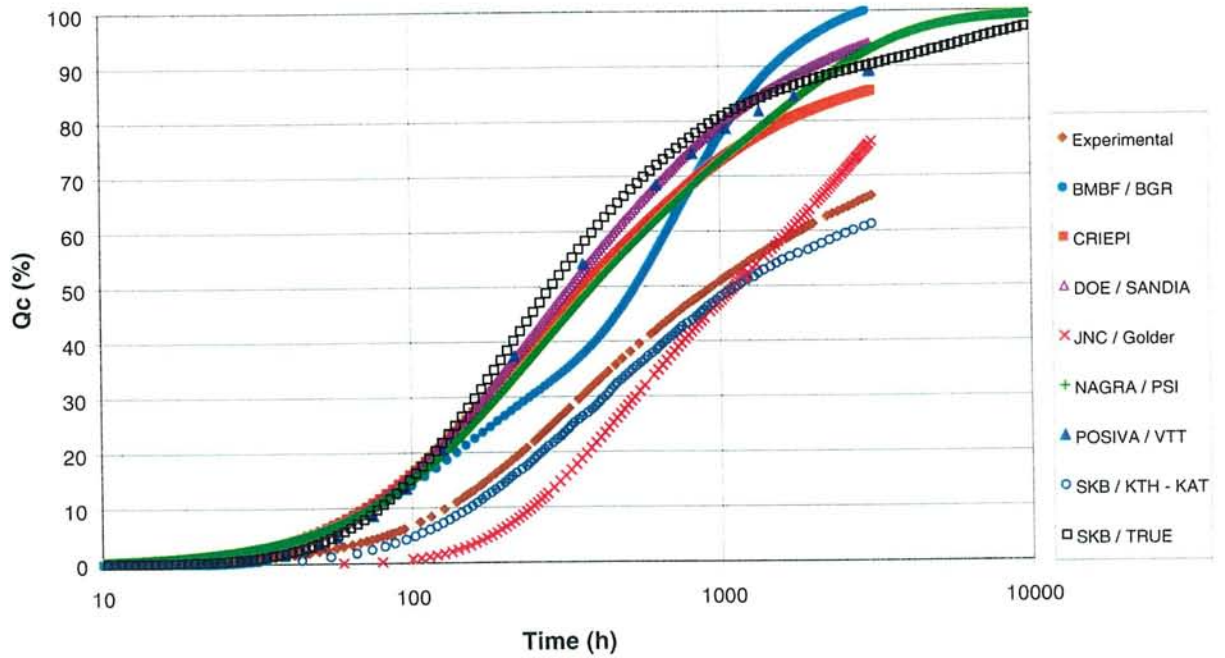
### TRUE-1 STT-2 Breakthrough Curves for Uranine



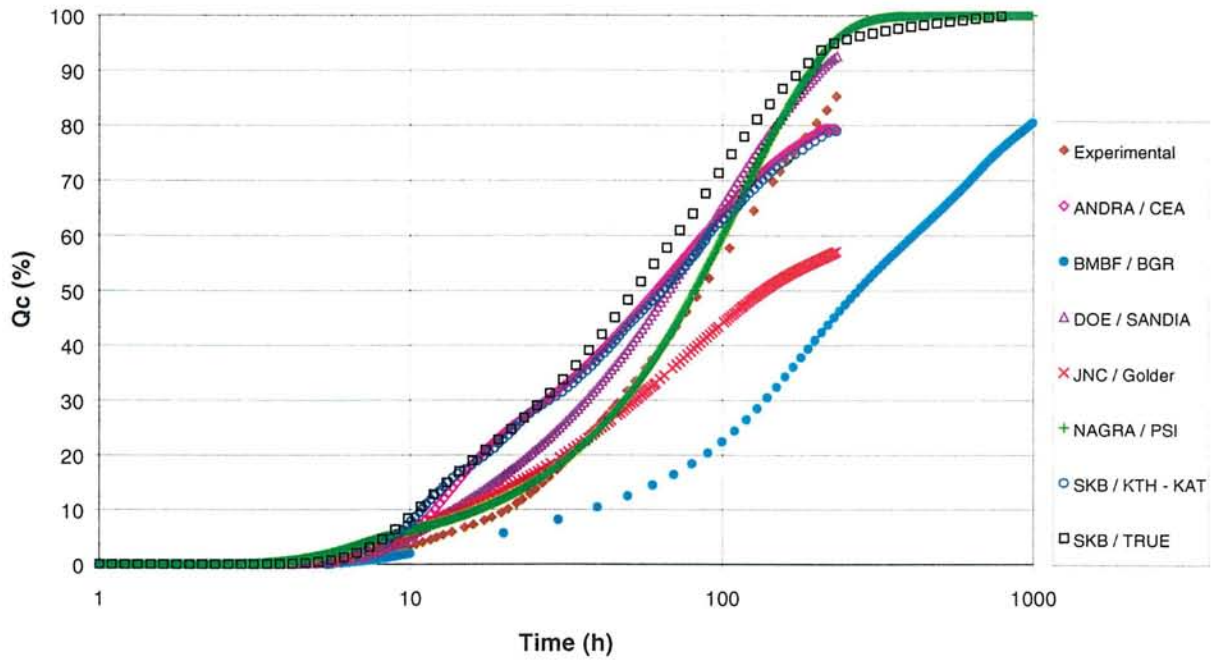
### TRUE-1 STT-2 Breakthrough Curves for Ba-131



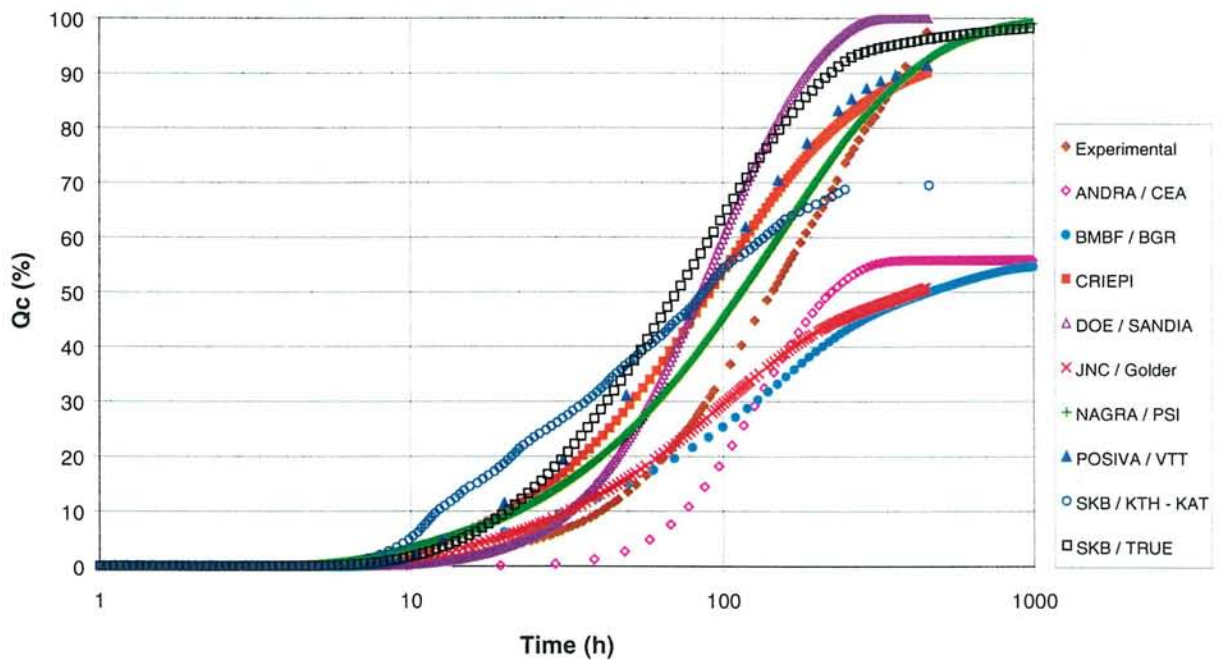
### TRUE-1 STT-2 Breakthrough Curves for Ba-133



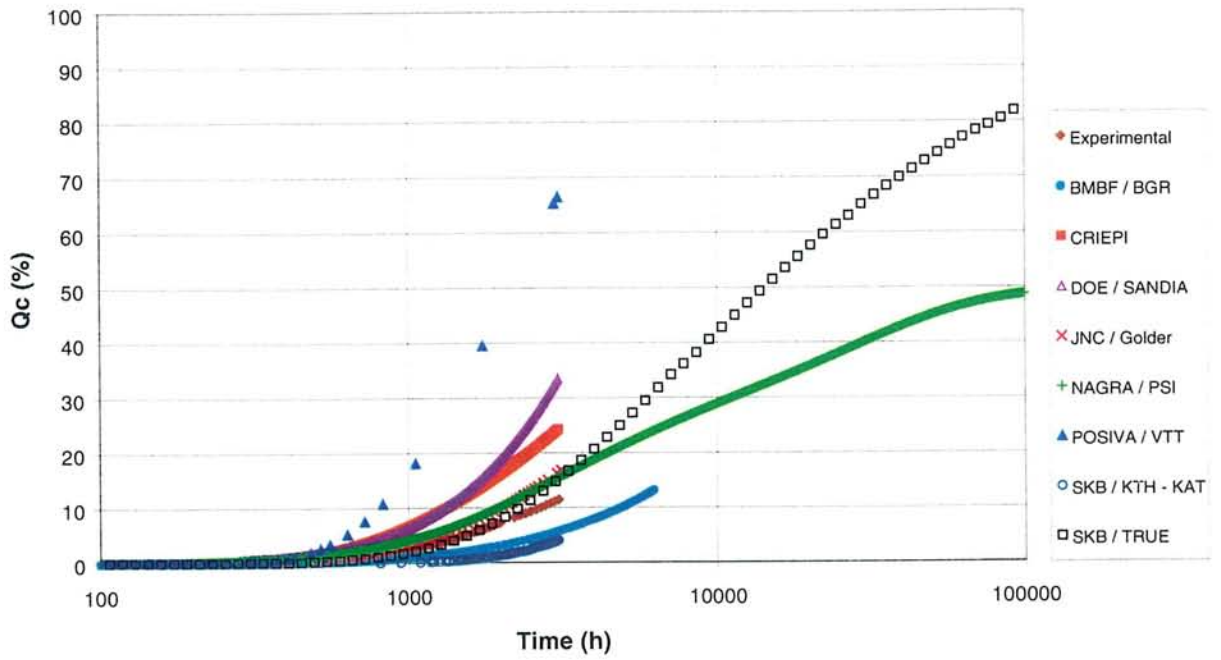
### TRUE-1 STT-2 Breakthrough Curves for Br-82



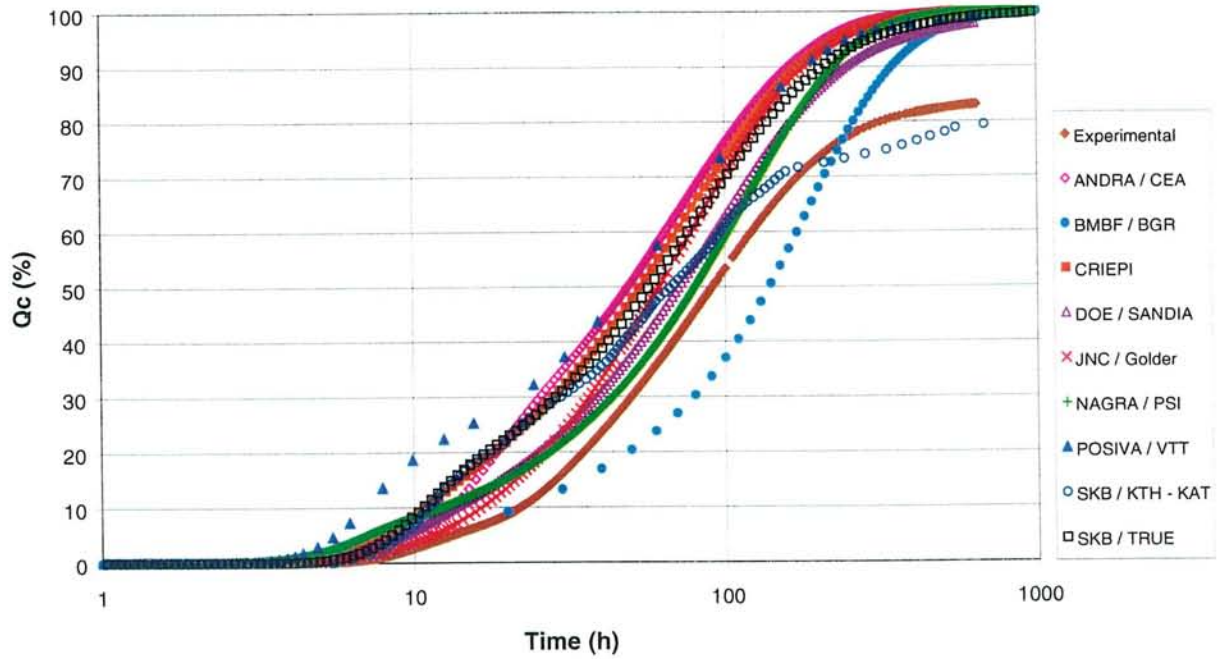
### TRUE-1 STT-2 Breakthrough Curves for Ca-47



### TRUE-1 STT-2 Breakthrough Curves for Cs-134

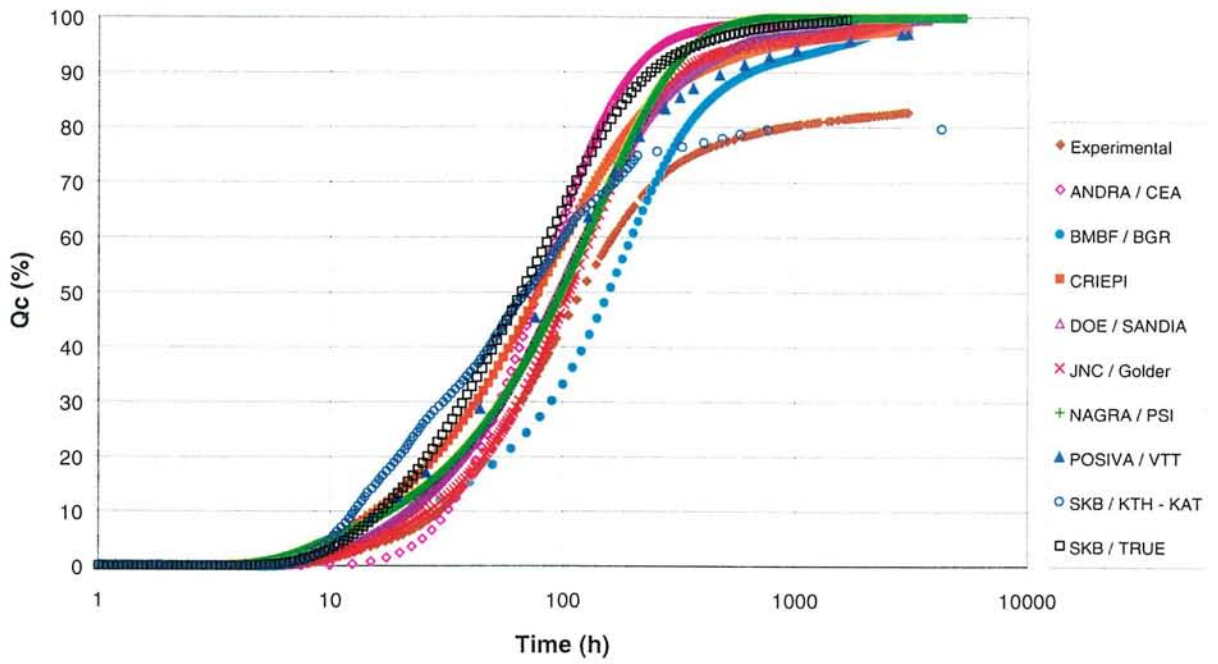


### TRUE-1 STT-2 Breakthrough Curves for Tritiated Water

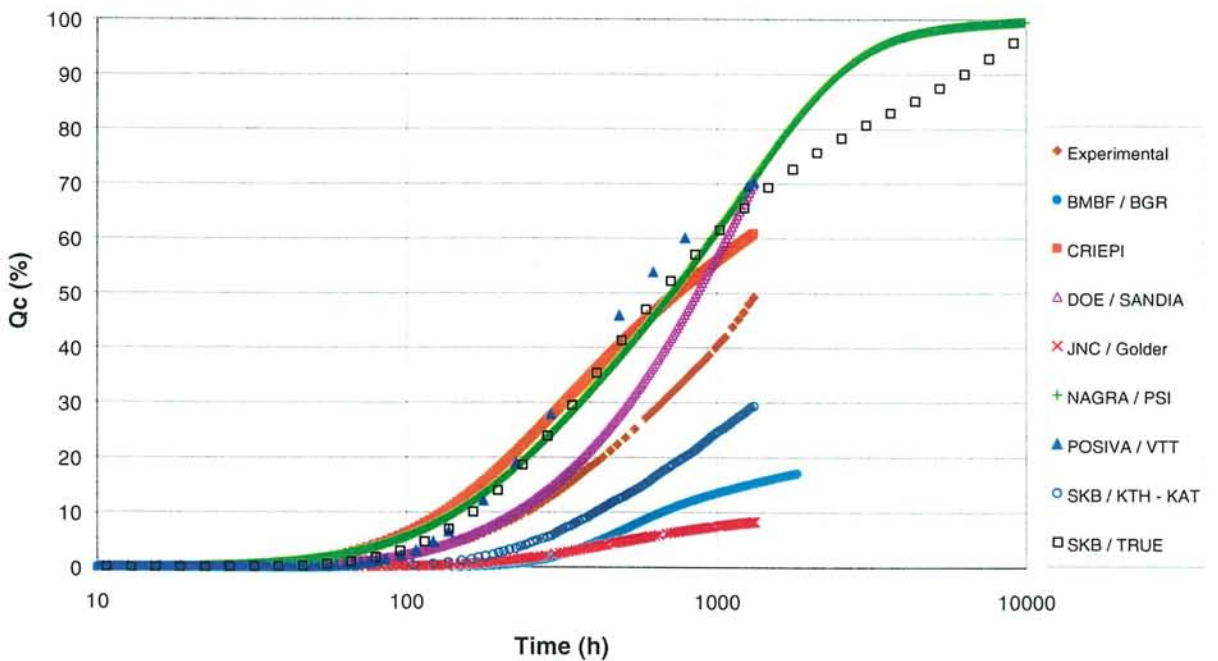




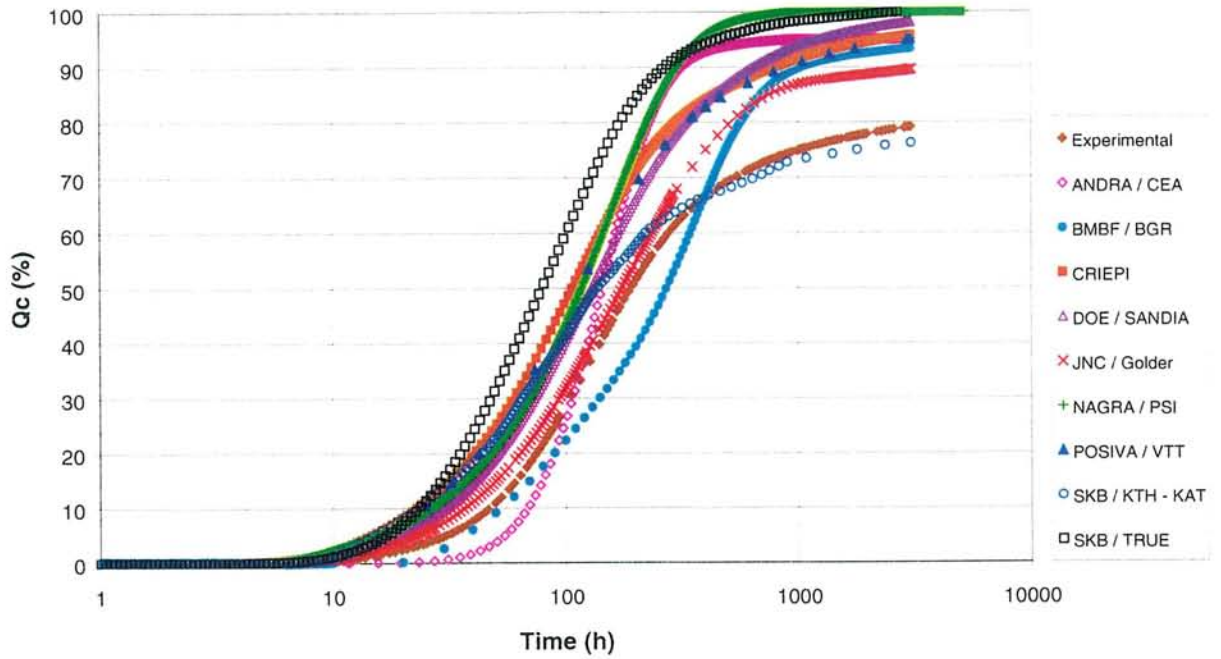
### TRUE-1 STT-2 Breakthrough Curves for Na-22



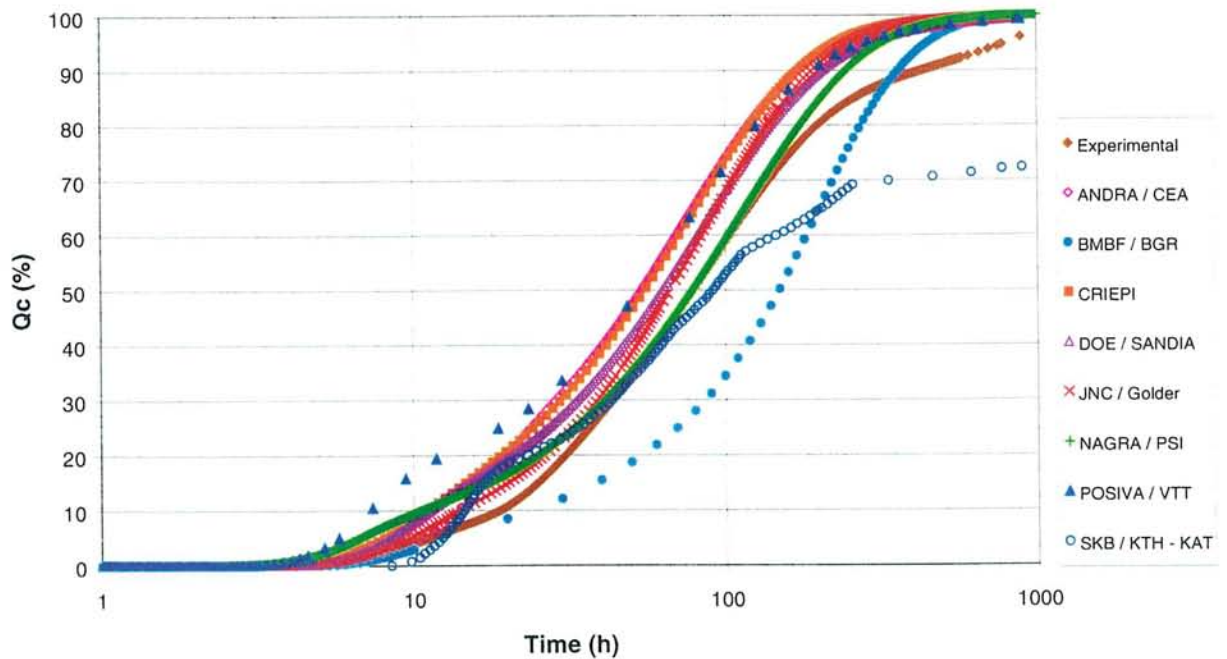
### TRUE-1 STT-2 Breakthrough Curves for Rb-86



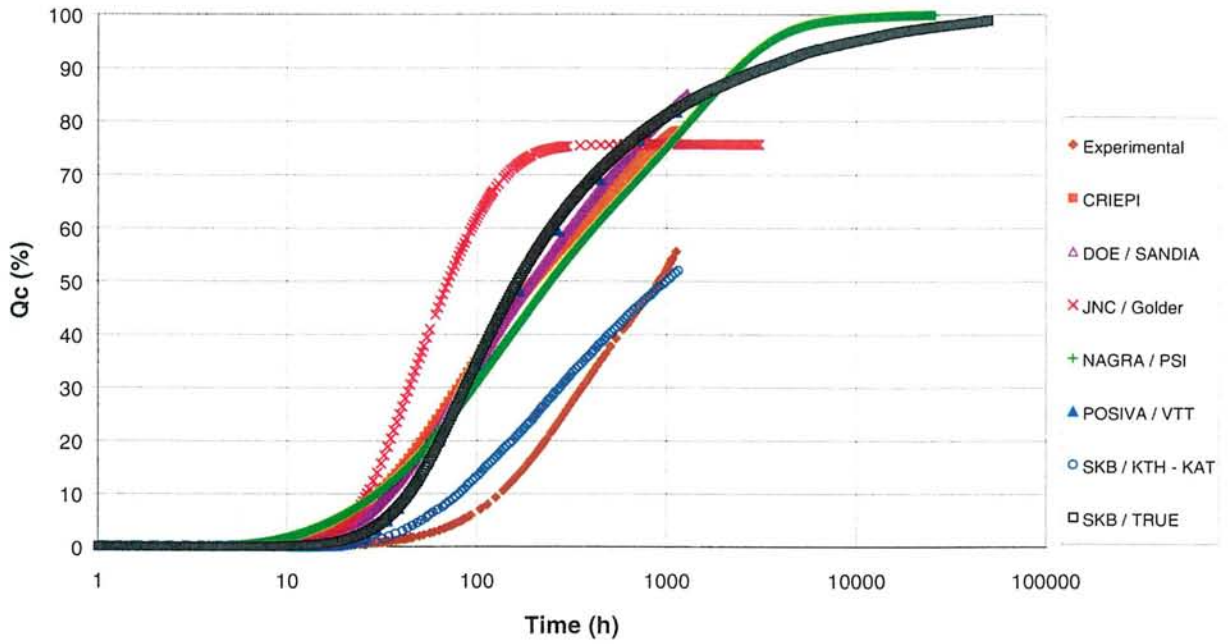
### TRUE-1 STT-2 Breakthrough Curves for Sr-85



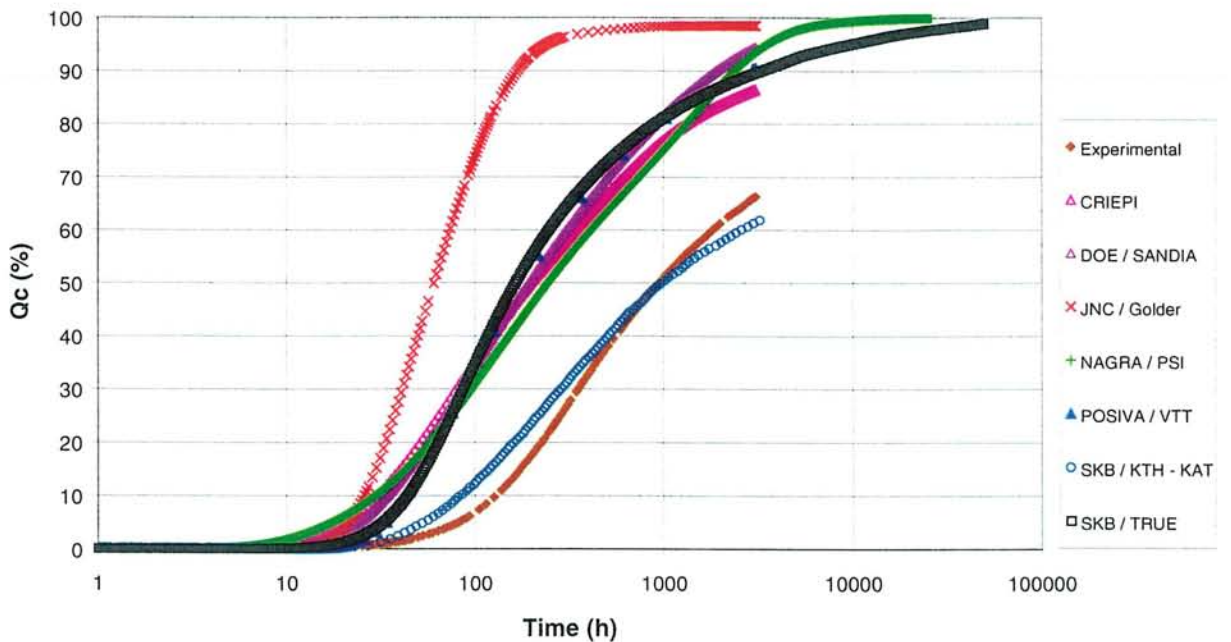
### TRUE-1 STT-2 Breakthrough Curves for Uranine



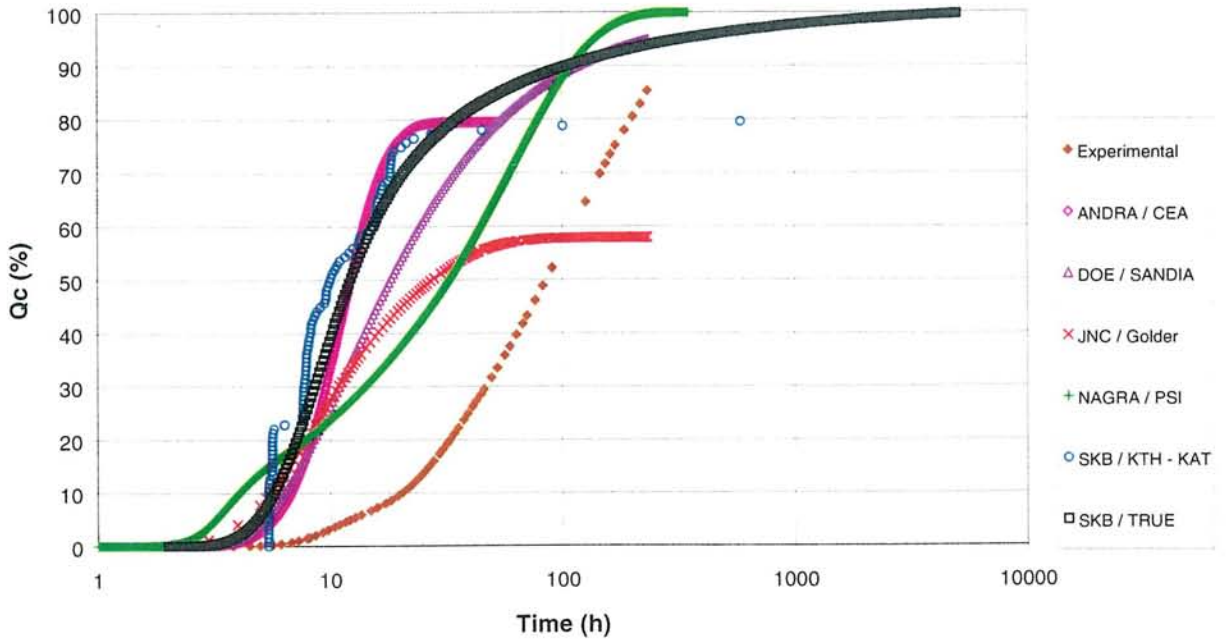
TRUE-1 STT-2 Breakthrough Curves for Ba-131: DIRAC Pulse Modelling, Stochastic/Deterministic Determination and Experimental Results



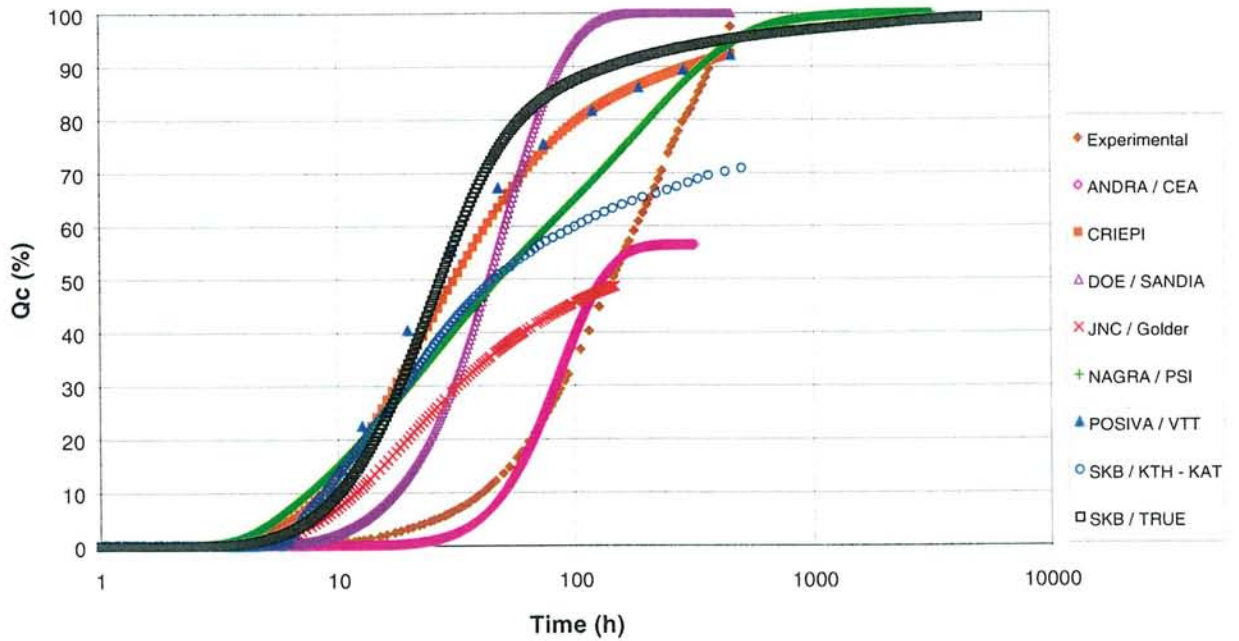
TRUE-1 STT-2 Breakthrough Curves for Ba-133: DIRAC Pulse Modelling, Stochastic/Deterministic Determination and Experimental Results



TRUE-1 STT-2 Breakthrough Curves for Br-82: DIRAC Pulse Modelling, Stochastic/Deterministic Determination and Experimental Results

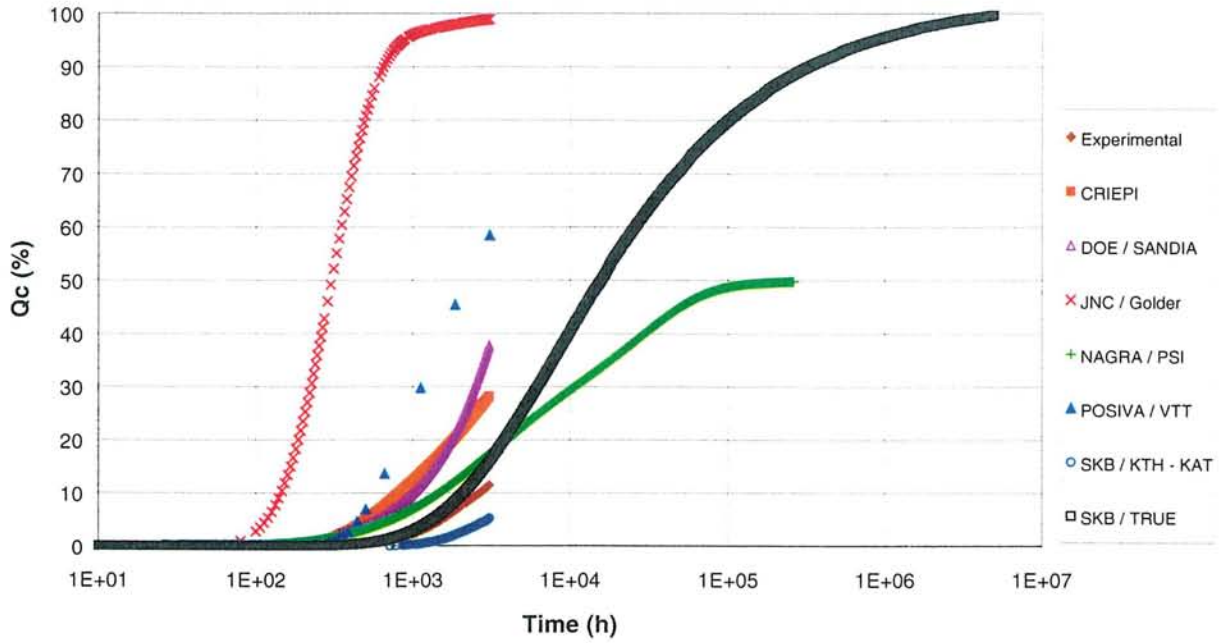


TRUE-1 STT-2 Breakthrough Curves for Ca-47: DIRAC Pulse Modelling, Stochastic/Deterministic Determination and Experimental Results

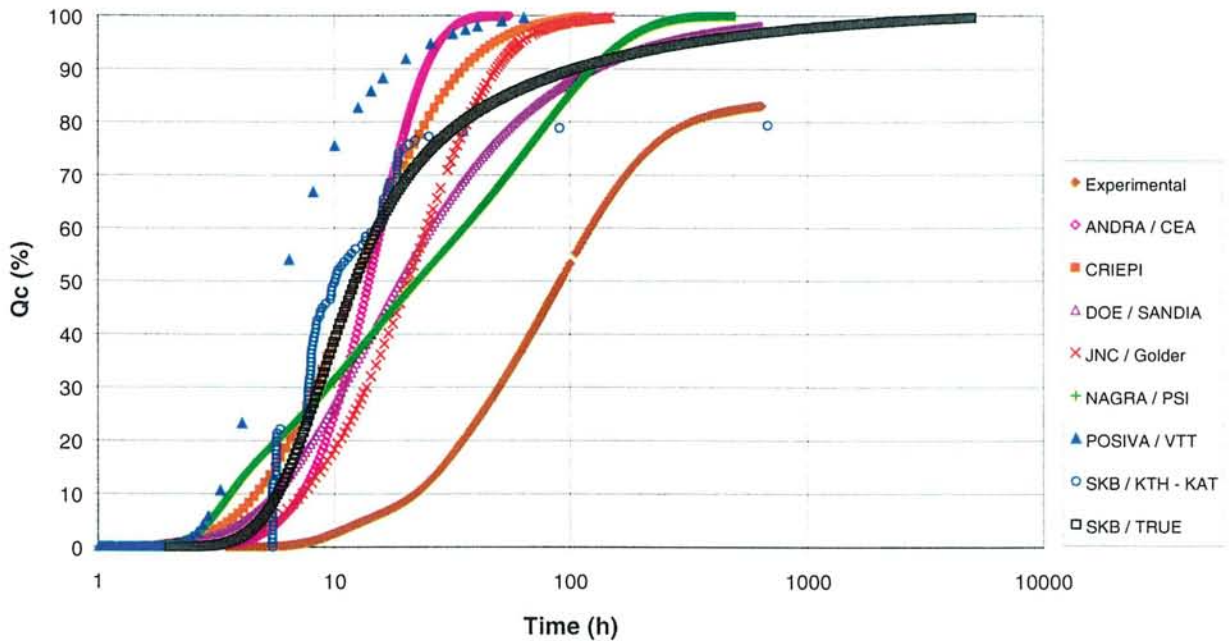




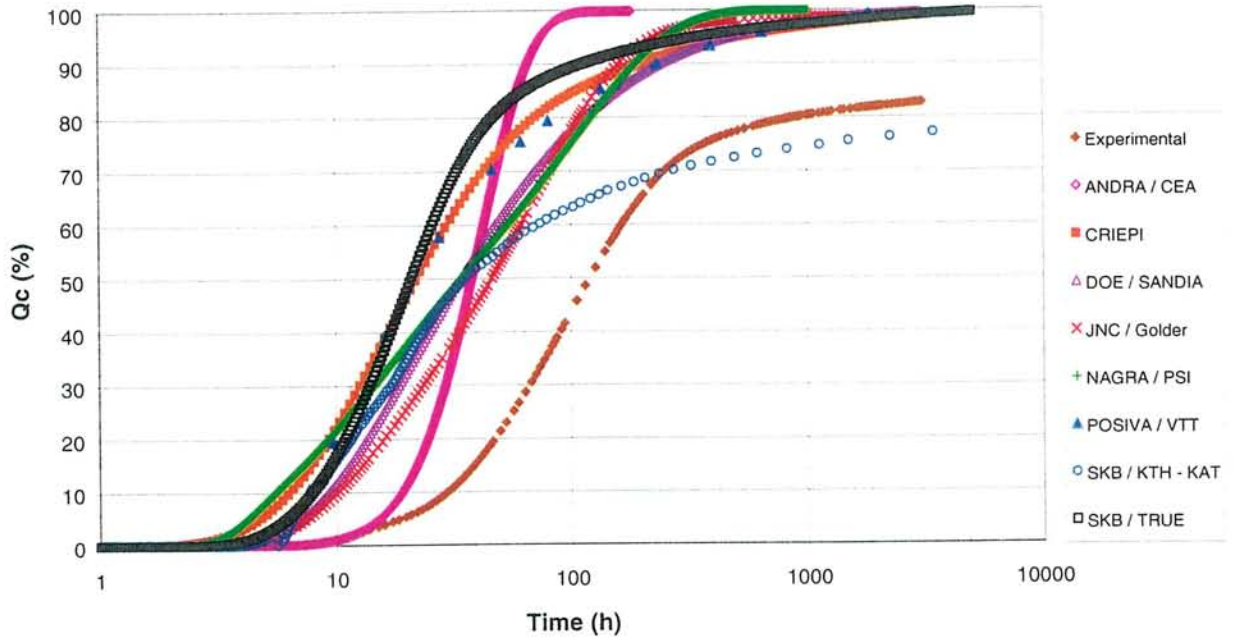
TRUE-1 STT-2 Breakthrough Curves for Cs-134: DIRAC Pulse Modelling, Stochastic/Deterministic Determination and Experimental Results



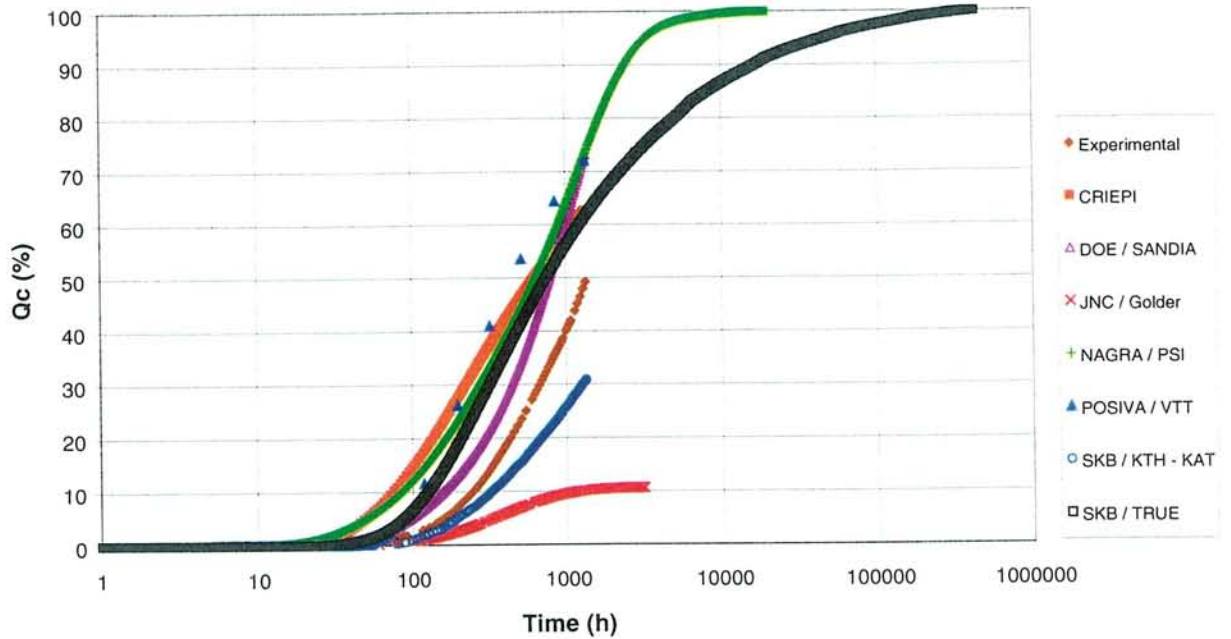
TRUE-1 STT-2 Breakthrough Curves for HTO: DIRAC Pulse Modelling, Stochastic/Deterministic Determination and Experimental Results



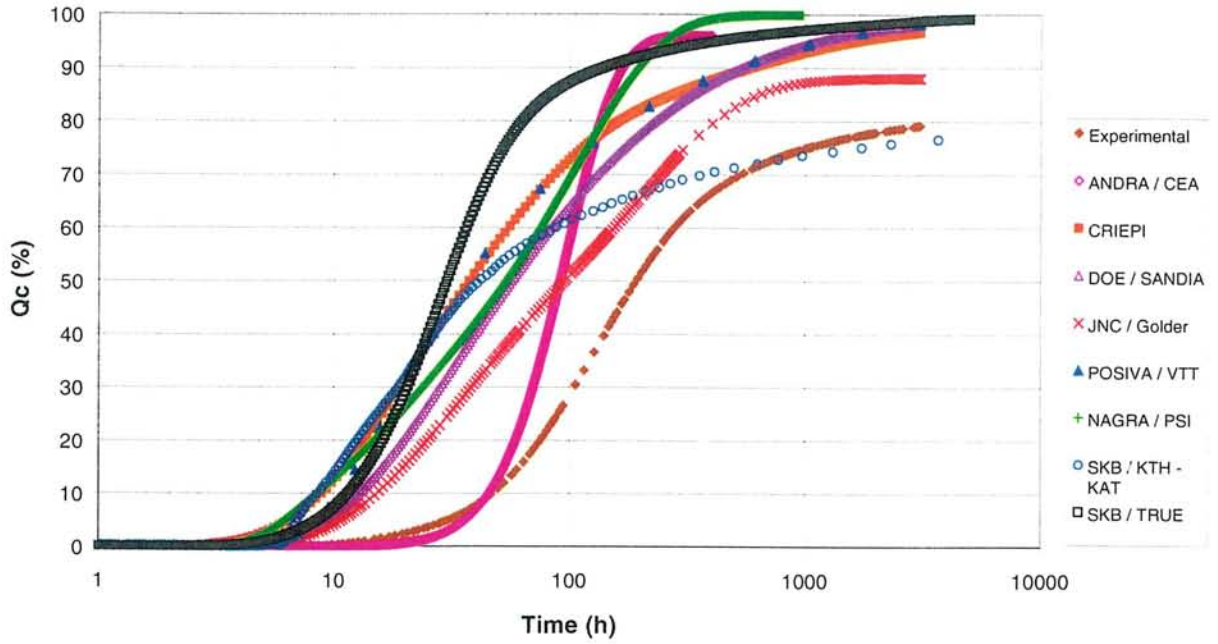
TRUE-1 STT-2 Breakthrough Curves for Na-22: DIRAC Pulse Modelling, Stochastic/Deterministic Determination and Experimental Results



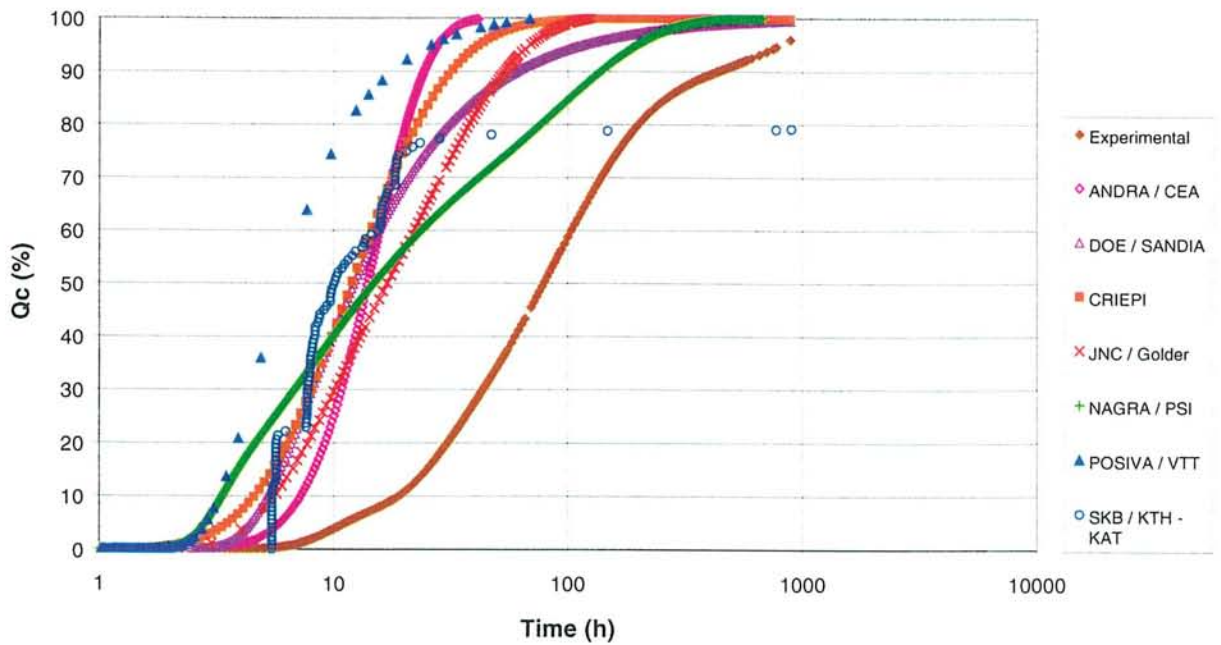
TRUE-1 STT-2 Breakthrough Curves for Rb-86: DIRAC Pulse Modelling, Stochastic/Deterministic Determination and Experimental Results



TRUE-1 STT-2 Breakthrough Curves for Sr-85: DIRAC Pulse Modelling, Stochastic/Deterministic Determination and Experimental Results



TRUE-1 STT-2 Breakthrough Curves for Uranine: DIRAC Pulse Modelling, Stochastic/Deterministic Determination and Experimental Results





## **B.2 Task 4C and 4D Evaluation**



## **Evaluation of Task 4C and 4D.**

M. Elert (SKB/Kemakta)





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# Evaluation of modelling of TRUE-1 RC and DP test Tasks 4C and 4D

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Äspö Task Force meeting 20 April 1999

Mark Elert

*Kemakta Konsult*

Kemakta

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## Introduction

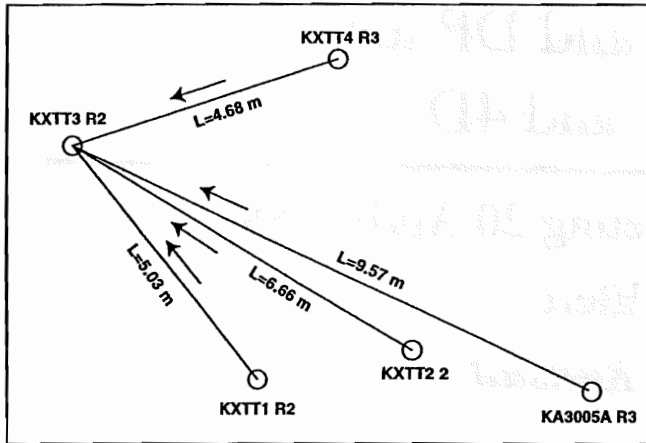
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- Based on:
  - ICR-reports
  - Modelling Questionnaire
  - Questionnaire on data usage
- Evaluation report now in print
- Contents:
  1. Introduction
  2. Purpose and set up of experiment
  3. Modelling approaches
  4. Results
  5. Discussion
  6. Conclusions

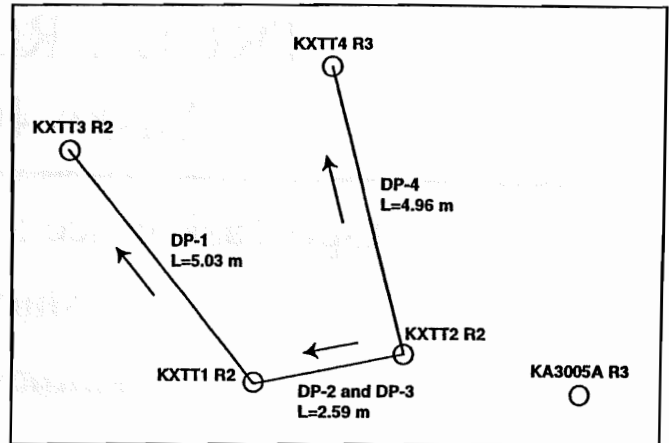
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# Experiments

## Radially converging test - RC



## Dipole tests - DP



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# Modelling approaches

- Types of models
  - Deterministic homogeneous
  - Deterministic heterogeneous
  - Stochastic continuum
  - Discrete Fracture Network
  - Channel Network
- Model geometry
  - Most groups considered Feature A as an isolated feature
  - PNC/Golder: Discrete Fracture Network
  - BMBF/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)

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# Data usage

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- **Transmissivities**
  - Deterministic models
    - preliminary tracer test
  - Stochastic models
    - pressure build-up tests
    - interference tests
    - preliminary tracer test
- **Boundary conditions**
  - head 10 - 15 m unaffected by pumping
    - hydrostatic head or
    - extrapolation of heads in boreholes before experiment
  - variations of boundary conditions
- **Model calibration and conditioning**
  - RC test predictions calibrated on Preliminary Tracer test
  - DP test predictions calibrated on RC test

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# Lessons learned

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- **Experimental site characterisation:**
  - generally thought to be good (presentation of data could be improved)
  - improvements for characterisation of head distribution, boundary conditions and connectivity structure
- **Experimental design:**
  - source term (improved methods for subsequent tests)
- **Performance measures:**
  - definition of accuracy measure (error in prediction) should be revised
  - relative measure (not absolute) for spread in time
- **Suggestions for additional data and analysis:**
  - more detailed analysis of hydraulic tests
  - additional head and flow measurements
  - spatial distribution of aperture (resin experiment)

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# Conclusions

## Tasks 4C and 4D as a testing exercise

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- An impressive amount of modelling has been performed
- Predictions of RC-test (based on site characterisation and preliminary tracer test):
  - predicted drawdown far from experimental results
  - high accuracy in prediction of tracer breakthrough from the two closest injection points
  - the majority of models did not predict the lack of recovery from the two other boreholes
- Predictions of DP-test (also data from RC-test):
  - considerable improvements in predictions of mass recovery and drawdown in pumping well
  - reasonable accuracy in predictions of tracer breakthrough
- Sufficient understanding of the part of Feature A encompassed by KXTT3-KXTT4-KXTT1.

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# Conclusions

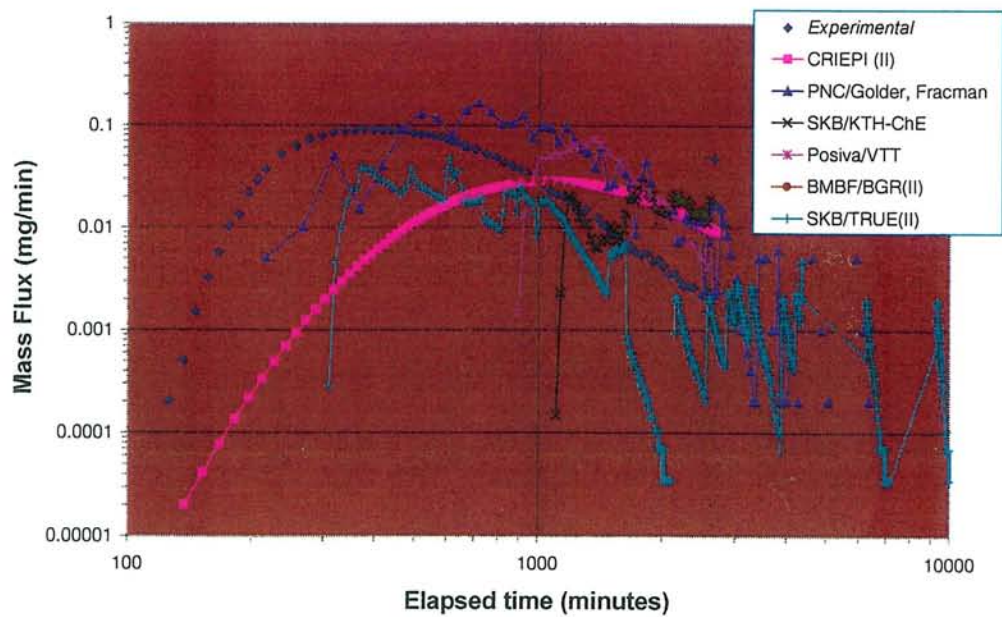
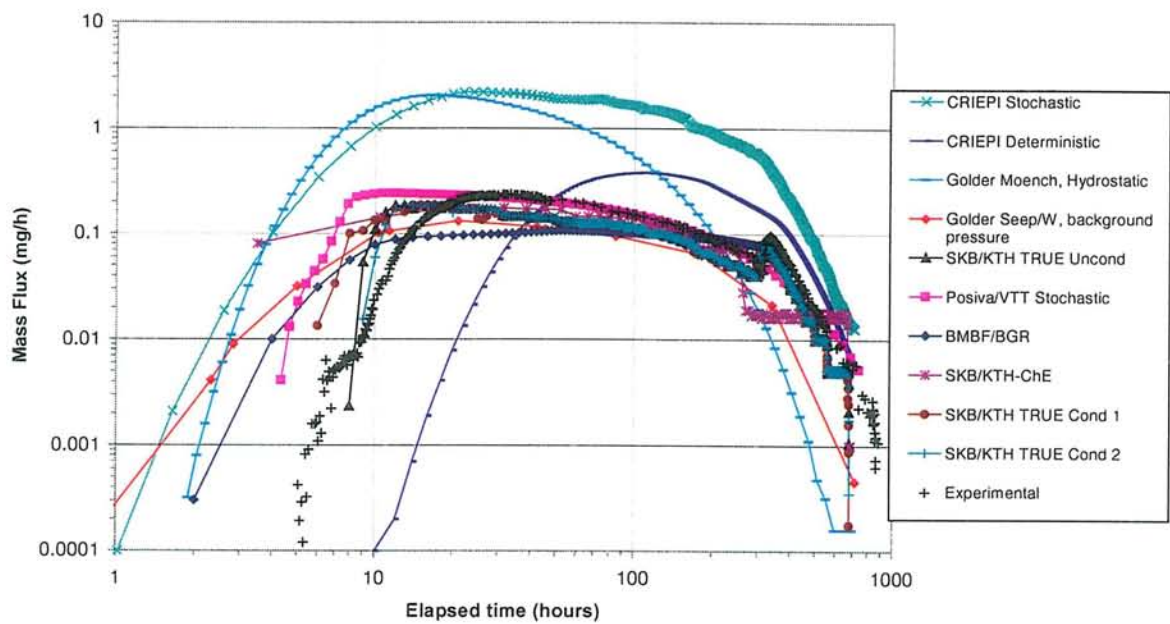
## Modelling and data

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- Feature A as a singular well-connected feature with limited connectivity
  - reasonable estimates obtained with relatively simple models
  - more elaborate models (e.g. using conditioning) required for more accurate predictions
- Beneficial to use models for evaluation of specific topics
- The general processes well understood, limited understanding of heterogeneity
- Need for suitable relationships between hydraulic aperture and transport aperture
- Boundary conditions
  - extrapolation to boundaries
  - changes with time
- The modelling teams did not use the data set from the site characterisation to its full extent (e.g. interference tests and pressure build-up tests)

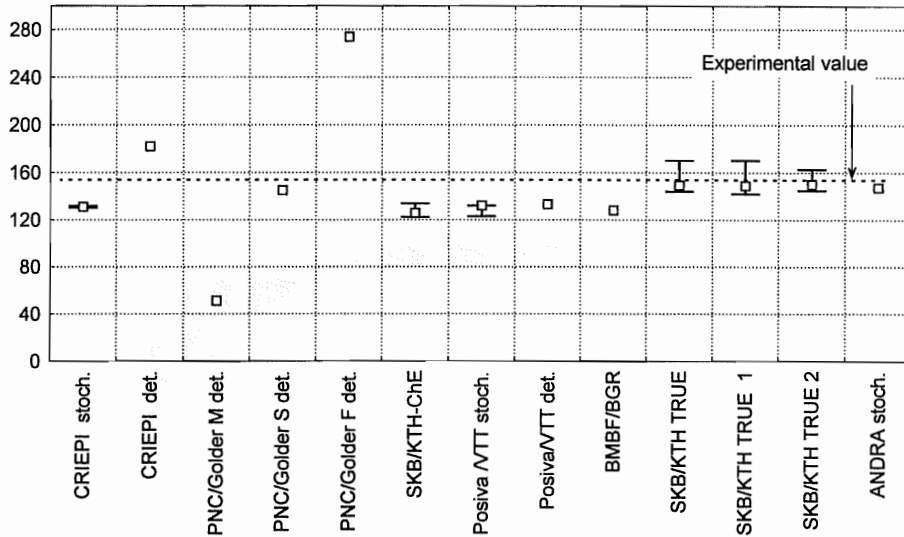
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# Breakthrough curves

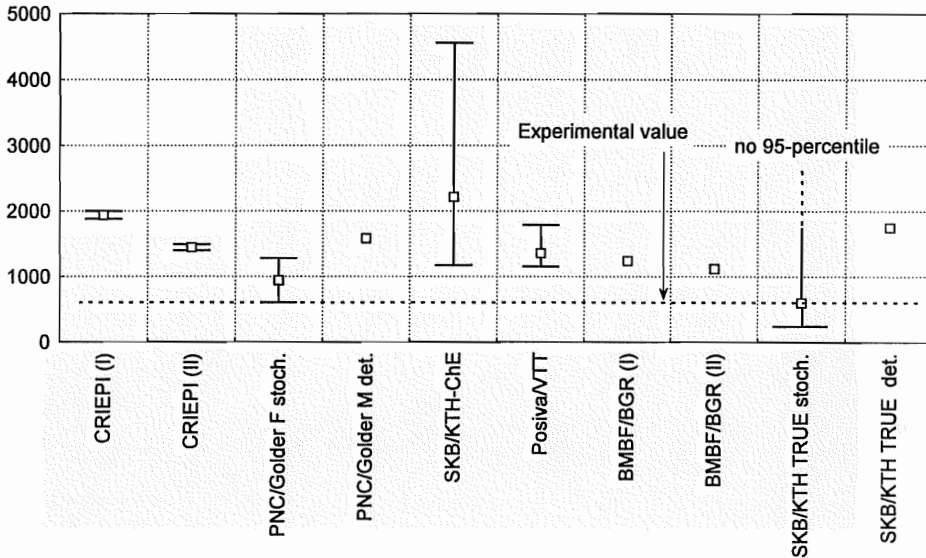


# Median breakthrough

RC-1 Test, Breakthrough times[h] for KXTT1, T50  
5%-, 50%- and 95% percentile for stochastic simulations

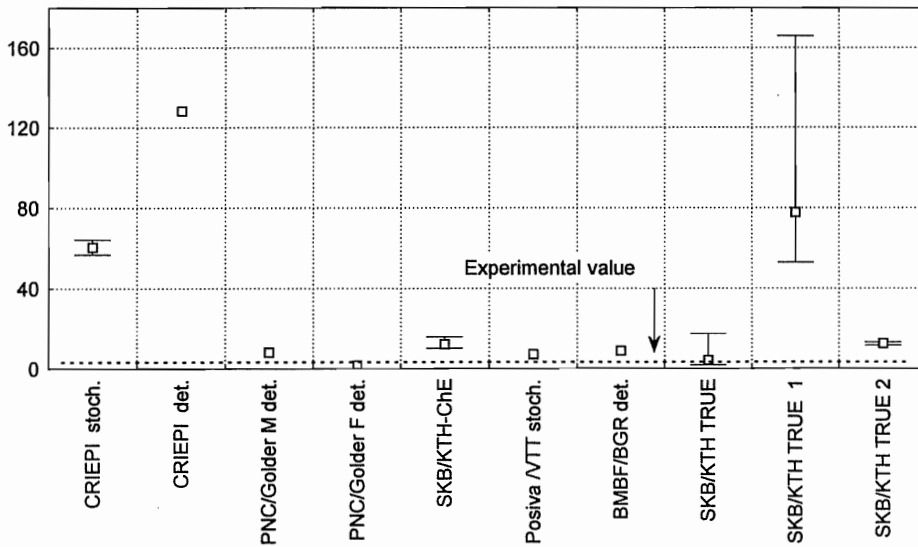


DP-1 Test, Breakthrough times [min], T50  
5%-, 50%- and 95% percentile for stochastic simulations

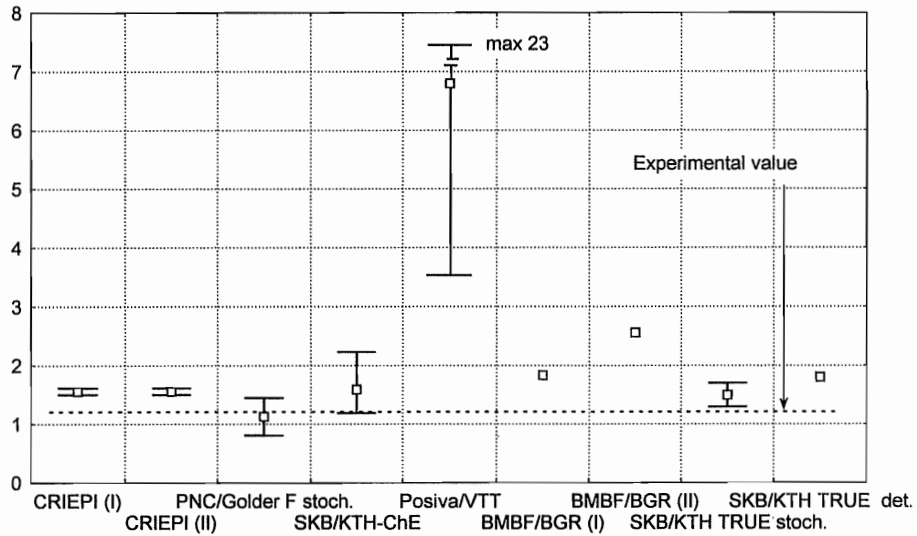


# Drawdown

RC-1 Test, Drawdown [m] for KXTT3:R2  
5%, 50% and 95% percentile for stochastic simulations



DP-1 Test, Drawdown [m] for KXTT3:R2  
5%, 50% and 95% percentile for stochastic simulations







## **Dirac modelling of STT1 & STT1b**

M. Elert (SKB/Kemakta)



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# Deconvolution of breakthrough curves STT-1 and STT-1b

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Äspö Task Force meeting 20 April 1999

Mark Elert and Håkan Svensson

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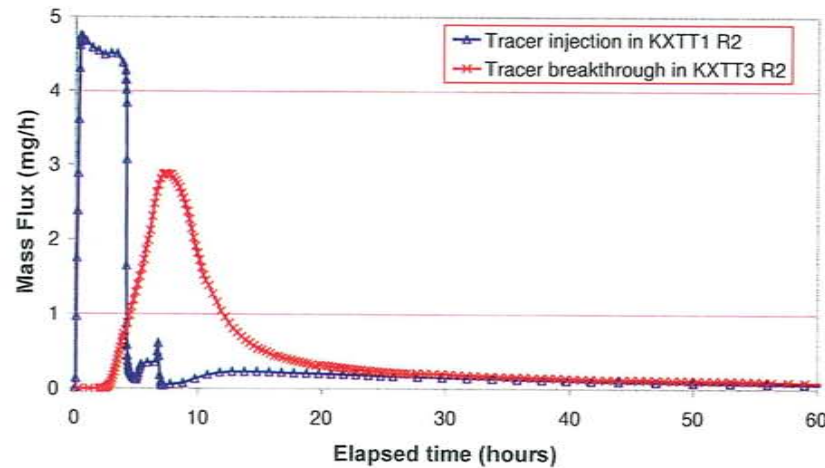
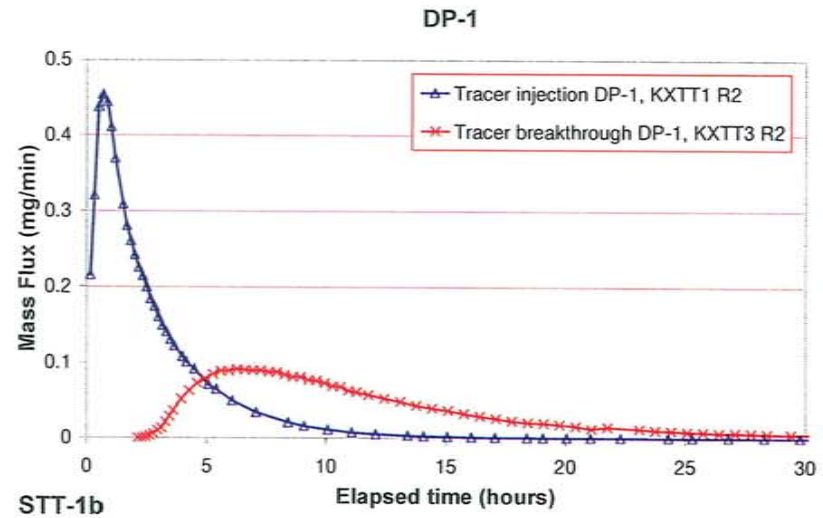
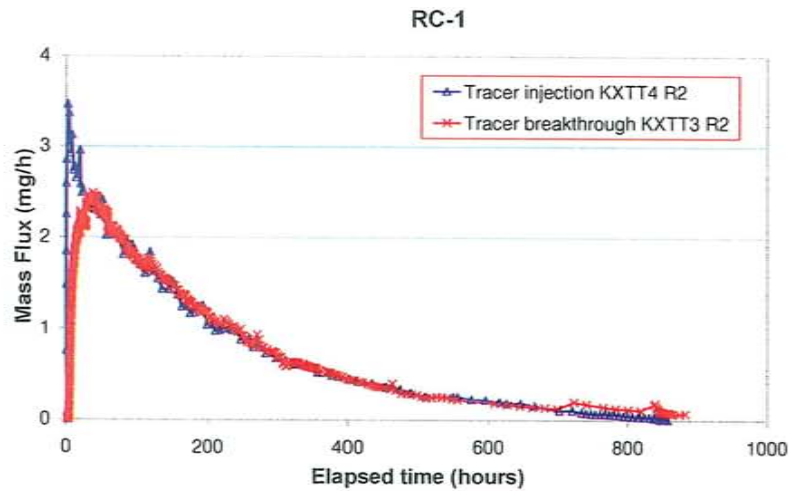
***Kemakta Konsult***

# Introduction

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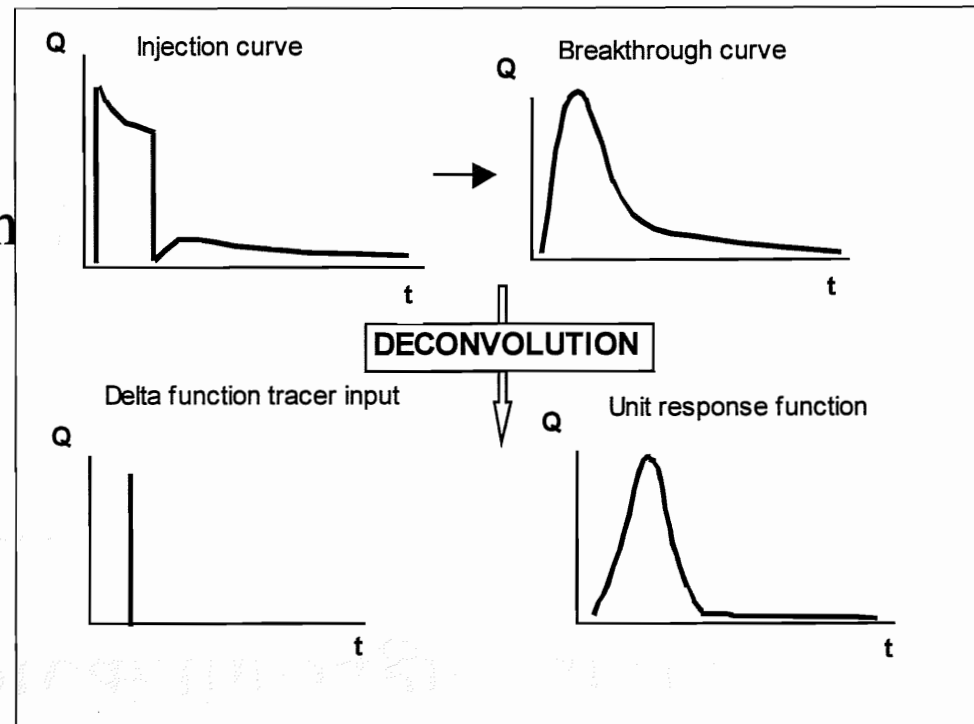
- Short well-defined injection source term beneficial for evaluation of tracer tests
- Practically difficult to achieve
- Evolution of injection techniques RC-DP-SST
- Mathematical treatment of experimental data -  
Deconvolution
  - eliminating the effect of the source term
  - problems with experimental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

# Injection and breakthrough curves

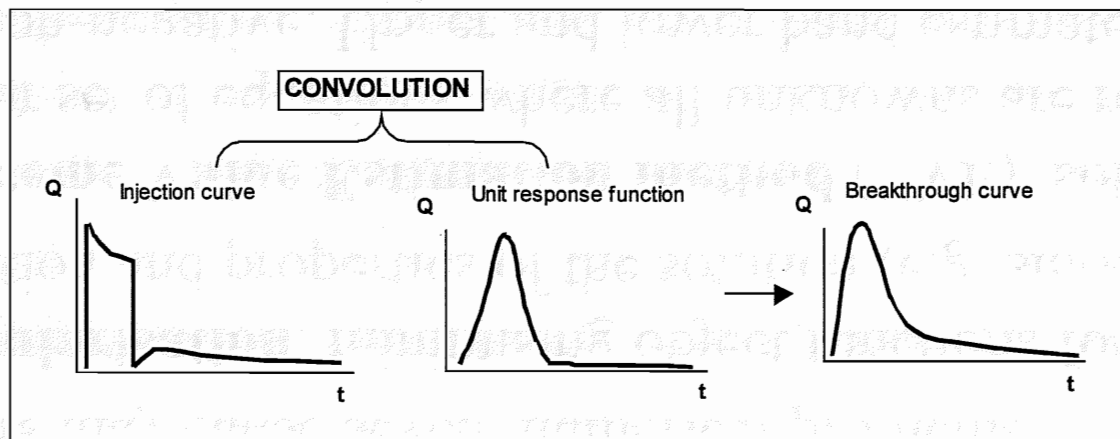


# Deconvolution

- 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)



# Convolution



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

# Deconvolution techniques

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- Deconvolution is an ill-posed problem: small measurement errors may cause severe numerical problems
- **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

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- 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.

$$M_i = \sum_j a_{ij} \cdot m_j$$

$$M_i = \sum_s m_{is} a_s$$

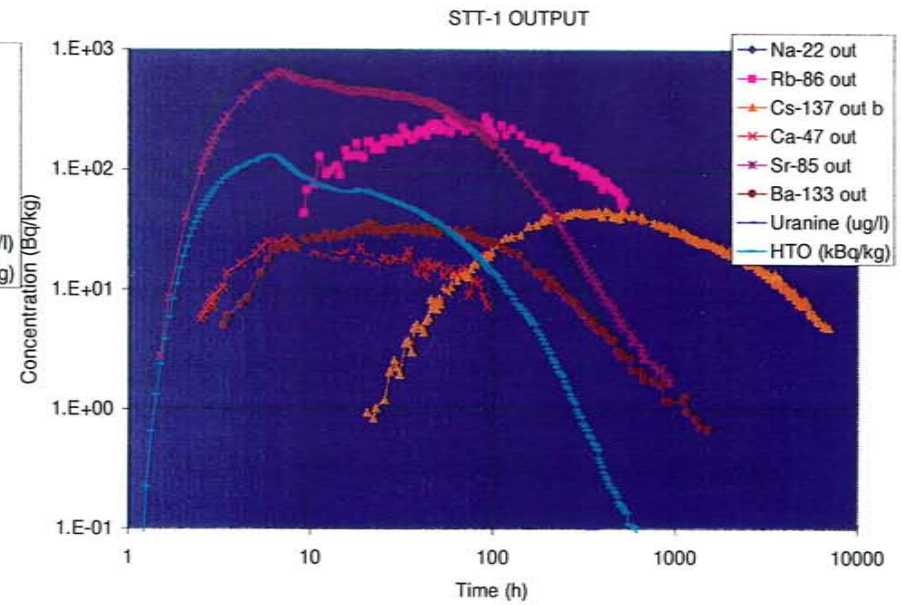
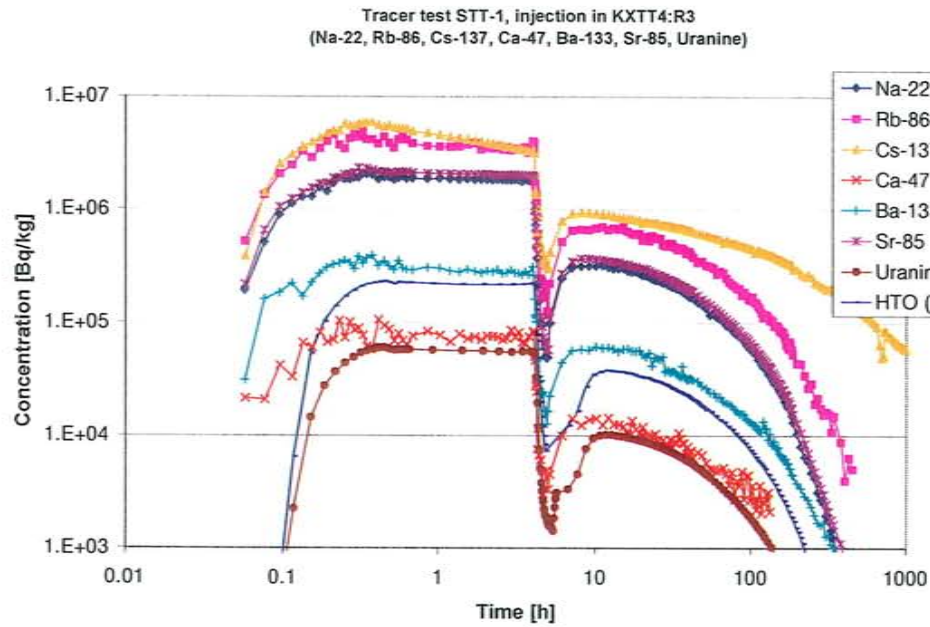
- **$M = m \cdot a$**
- **$a = m^{-1}M$**

## Method used in this study (contd.)

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- The Toeplitz method considerably more stable than deconvolution routine of Matlab
- Fitting of injection curves
  - injection curves divided into several parts and fitted to a simple function (linear, logarithmic, exponential)
- Filtering of breakthrough curves
  - spiky curves were filtered using a moving average filter
- Convolution of unit response function
  - the result was convoluted with the injection curve and compared with the original breakthrough curve

# Deconvolution of STT-1



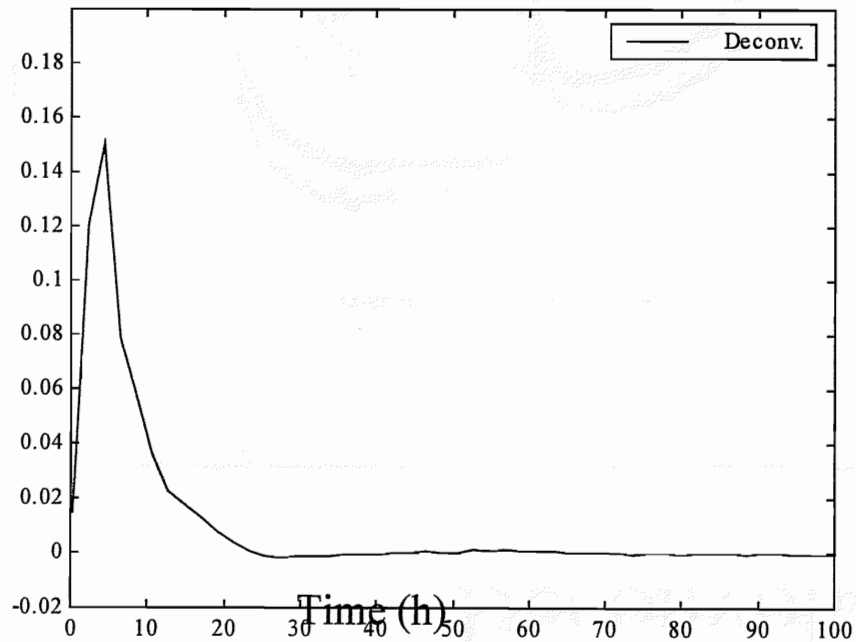
# Deconvolution of STT-1 (contd.)

**Time steps and methods used for deconvolution of the STT-1 test.**

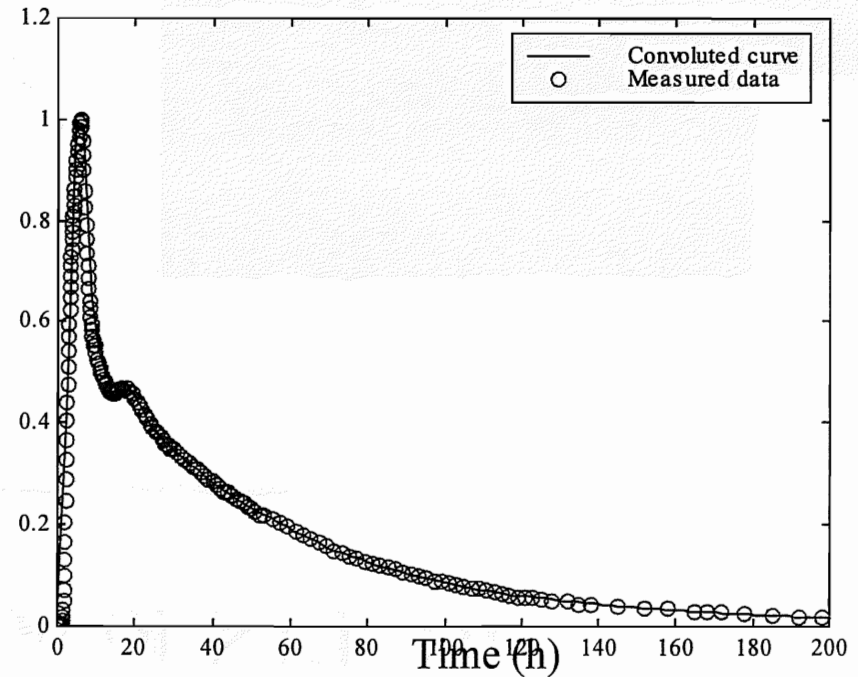
	<b>Start time (h)</b>	<b>Time step (h)</b>	<b>Injection curve</b>	<b>Breakthrough curve</b>
Uranine	0.21	2.1	exp	exp
HTO	0.13	2.01	exp	exp
Na-22	0.05	2.04	exp	exp
Sr-85	0.06	2.04	exp	exp
Ba-133	0.0001	2.05	curve- fitted	smoothed
Rb-86	0.05	2	curve- fitted	smoothed
Ca-47		Incomplete breakthrough curve		
Cs-137		Too long breakthrough curve		

# STT-1 Uranine

Unit reponse function (1/h)

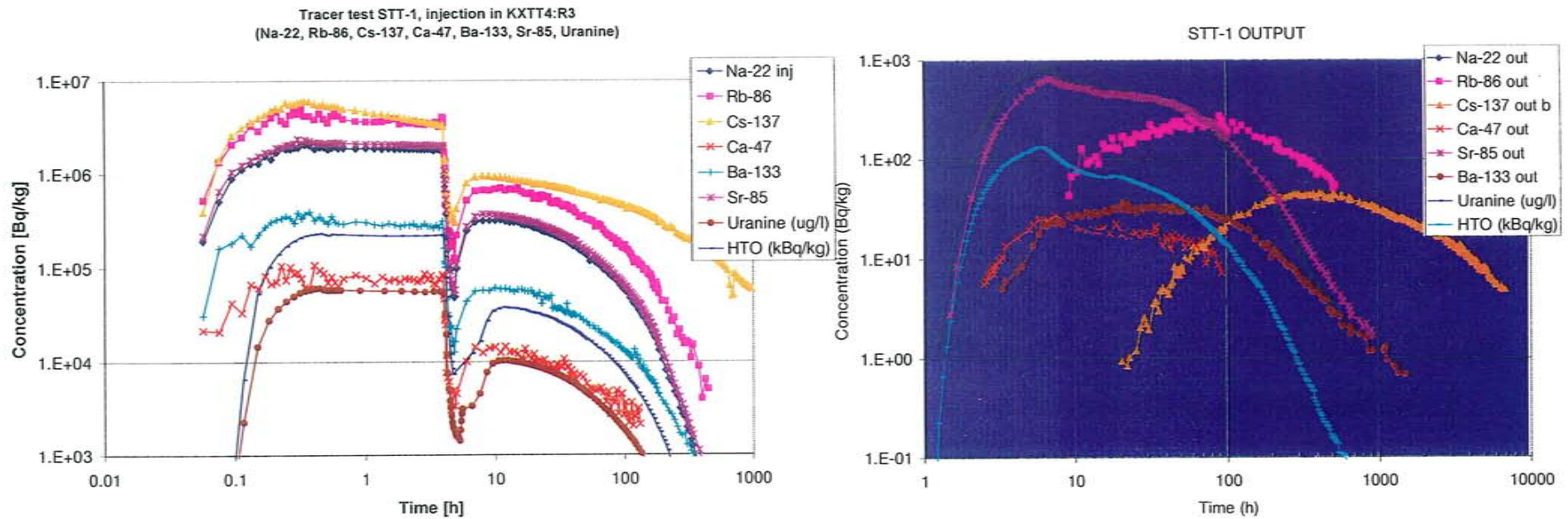


Convolutd curve and measured data (mg/h)



Kemakta

# Deconvolution of STT-1b



# Deconvolution of STT-1b (contd.)

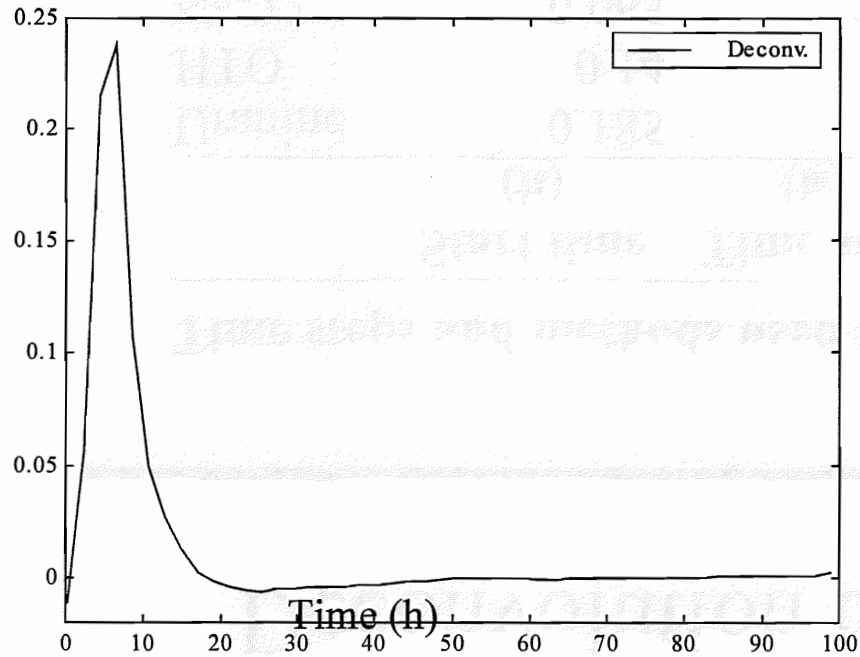
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**Time steps and methods used for deconvolution of the STT-1 test.**

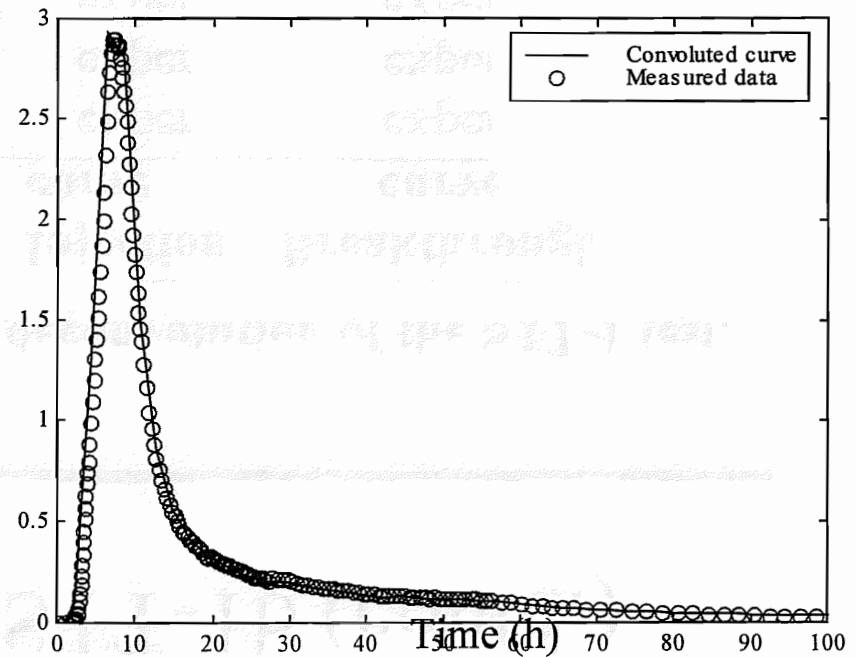
	<b>Start time (h)</b>	<b>Time step (h)</b>	<b>Injection curve</b>	<b>Breakthrough curve</b>
Uranine	0.185	2.1	exper	exper
HTO	0.14	2.	exper	exper
Na-22	0.065	2.04	exper	exper
Sr-85	0.06	2.04	exper	exper
Co-58	0.0001	2.5	exper	smoothed
Rb-86		Incomplete breakthrough curve		
K-42		Incomplete breakthrough curve		

# STT-1b Uranine

Unit reponse function (1/h)



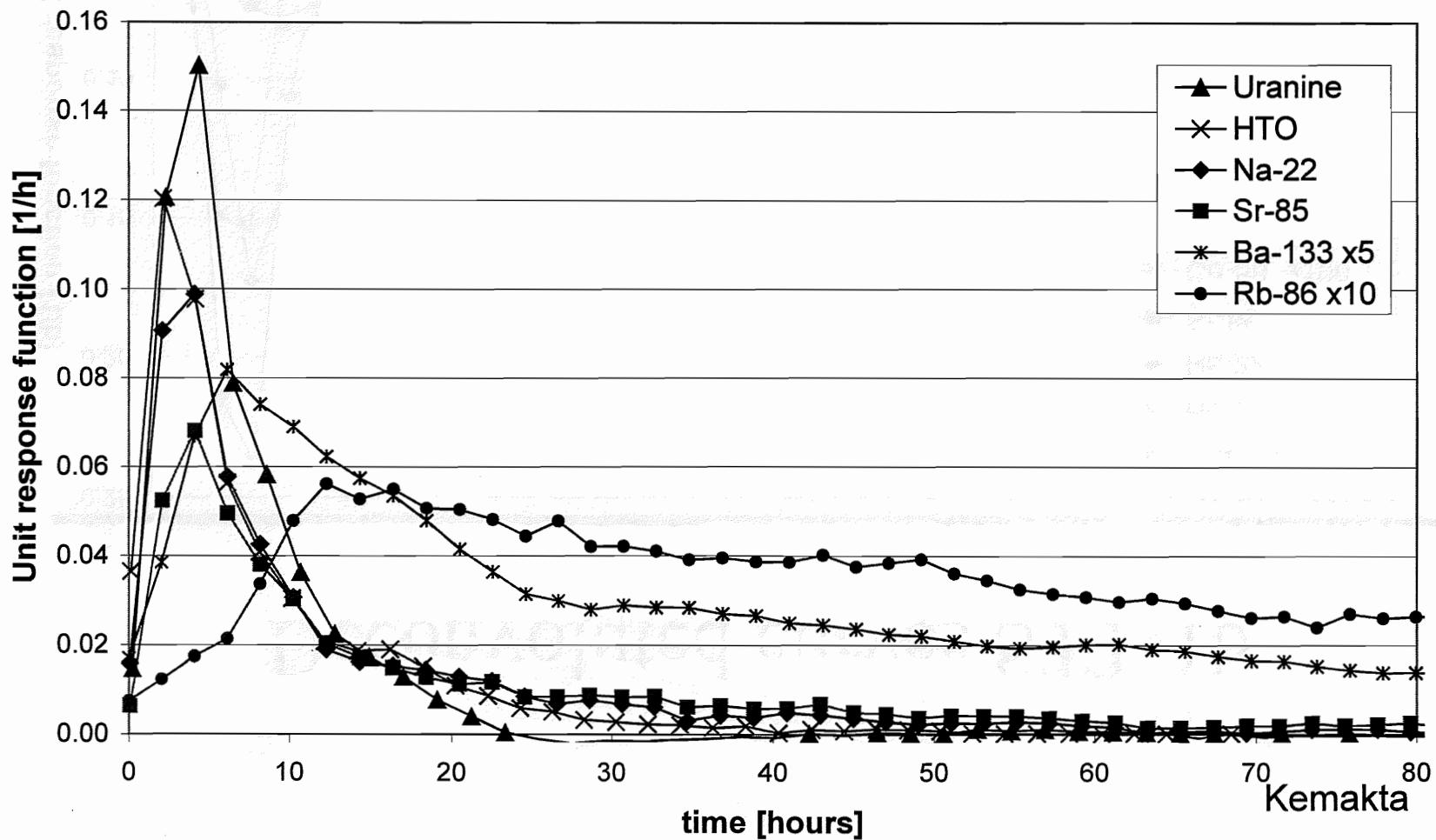
Convolutd curve and measured data (mg/h)



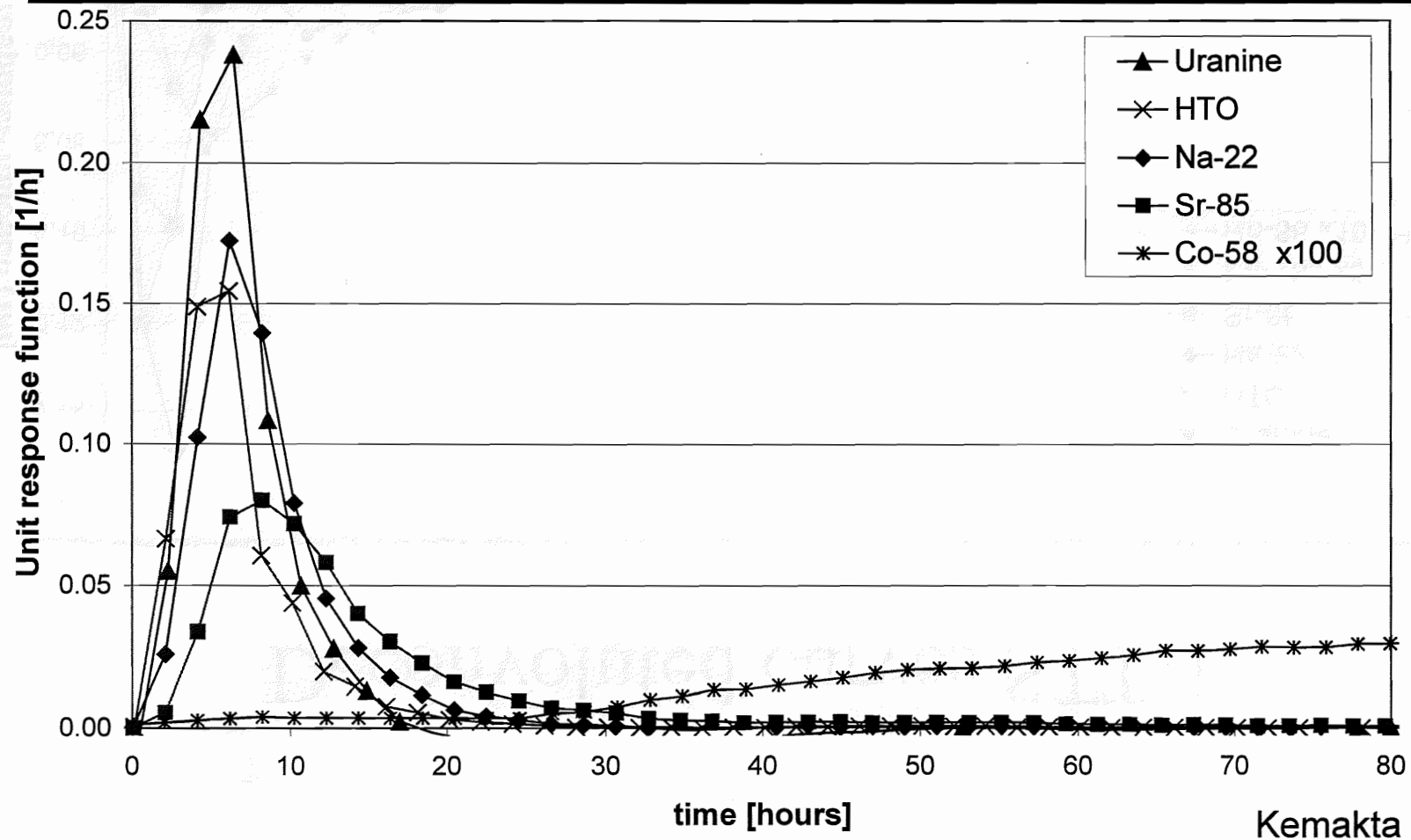
Kemakta



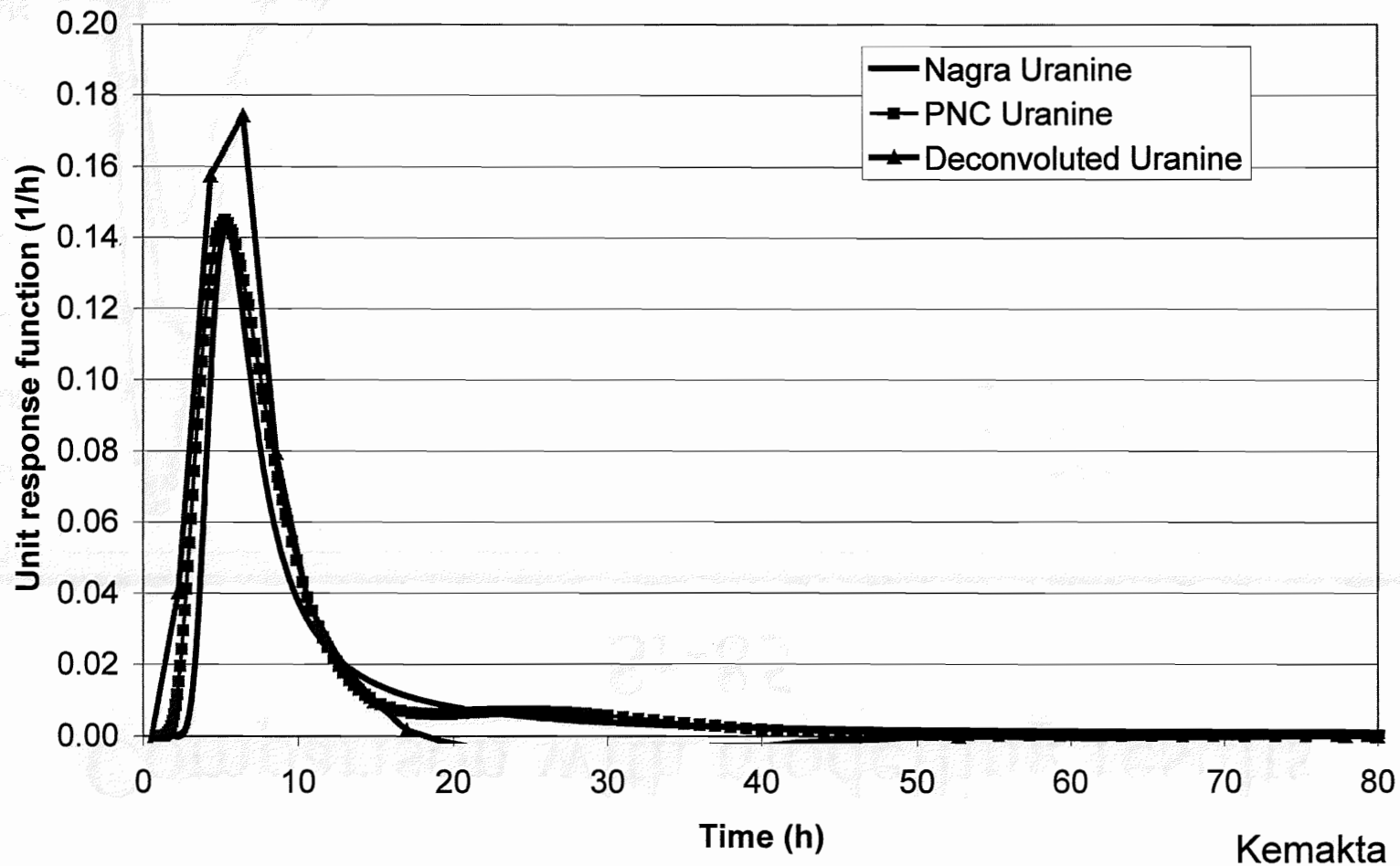
# Deconvoluted curves STT-1



# Deconvoluted curves STT-1b

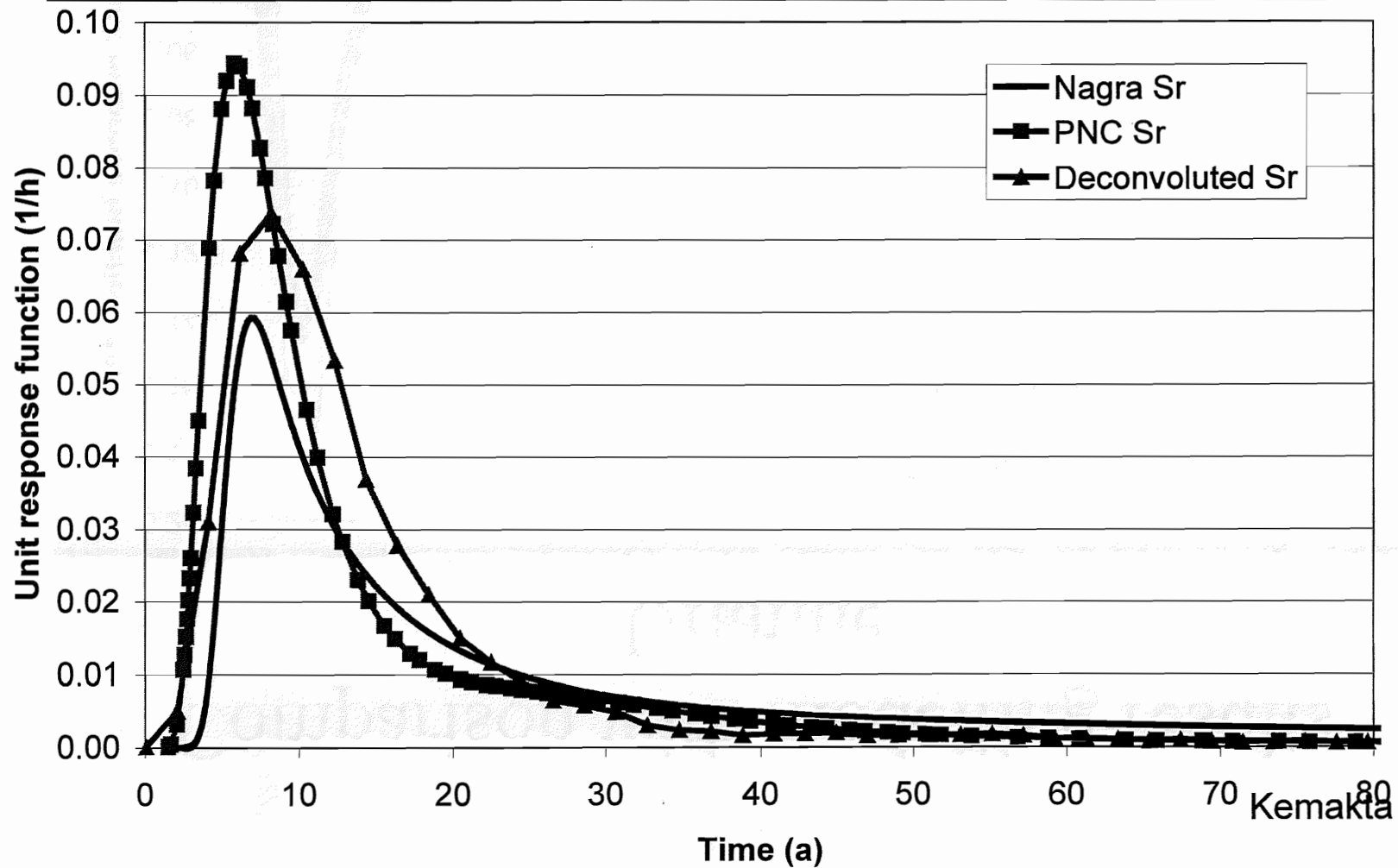


# Comparison with modelling results Uranine



# Comparison with modelling results

## Sr-85



# Conclusions

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- 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
- Present method has successfully deconvoluted most tracers used in STT-1 and STT-1b
- Areas for possible improvement
  - difficulties finding optimal constant time step
  - filtering of spiky output data
  - negative values appears
  - more automated optimisation

