International
Progress Report

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Äspö Hard Rock Laboratory

Äspö Task Force on modelling of groundwater flow and transport of solutes

Proceedings from the 14th Task Force meeting at Säröhus, Sweden, Nowember 14-16, 2000

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May 2001

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Äspö Hard Rock Laboratory

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

Abstract

This report summarises the main findings of the modelling work done by different modelling groups in the Task Force since the previous meeting and presented at the 14th Task Force meeting held 14-16 November, 2000 at Säröhus, Sweden. The report also constitutes a status report of the Task Force work. The subject of this report is the work performed in Task 4 dealing with solute transport in one structural featur at a 5m scale. The second modelling task ,Task 5, is a hydrological-hydrochemical model assessment exercise that specifically studies the impact of the tunnel construction on the groundwater system at Äspö. The scale of study is in the order of several hunbdred of meters.

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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 Radiactivas (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 14th Task Force meeting held 14-16 November, 2000 at Säröhus, Sweden. The report also constitutes a status report of the Task Force work. Tasks 1-3 have been completed and the subject of this report is the work performed in Task 4 and Task 5.

Reports produced within the framework of the Äspö Task Force published since the previous 13th 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.

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.

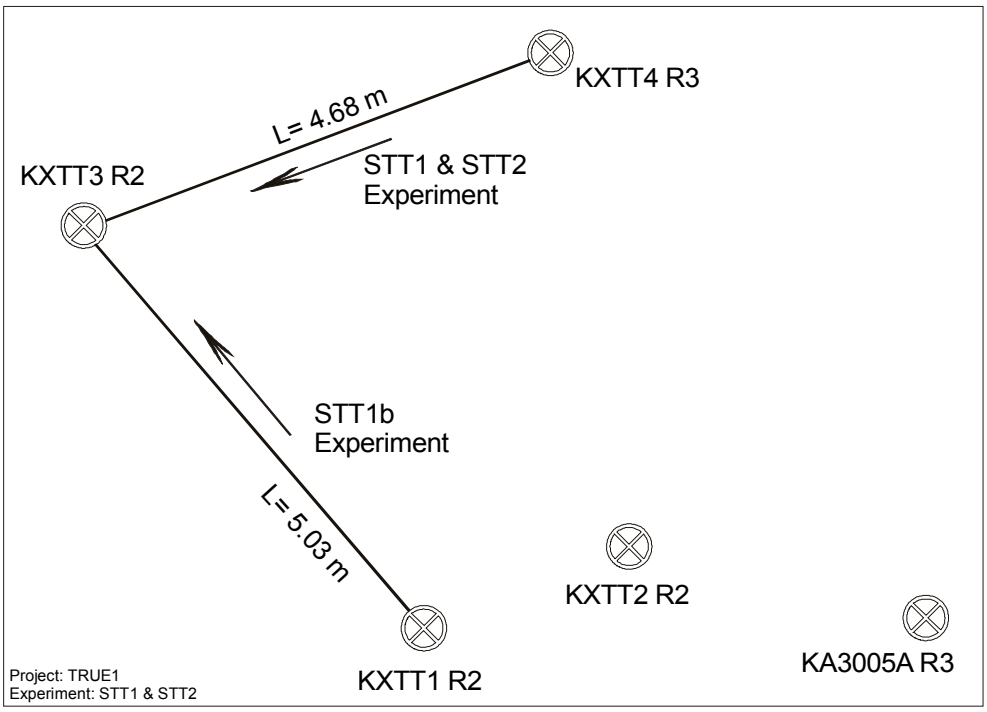

Figure 3-1 Borehole intersections with Feature A shown in the plane of the feature. Distances given in metres.

3.3 Results Task 4

Luis Moreno made an exercise on assuming 3D flow instead of 2D which resulted in a flow wetted surface being approximately 30 times larger than in 2D flow geometry, Appendix A.

Results were presented by Mark Elert on the compilation of modelling with Task 4E and 4F by all teams as well as evaluation of their work. (Appendix B).

The outcome of the Task 4F deconvolution exercise was also presented by Mark Elert, Appendix C.

All modelling performed within Task 4 shall be evaluated with respect to understanding, methodologies and motivation/expectations of the participating organisations. During the meeting a brainstorming on specific issues which could be potentially viable to include was initiated by Paul Marschall, Appendix D.

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 Äspö 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.

4.2 Work performed

A preliminary summary of the results obtained by the different modelling teams was compiled and presented by Ingvar Rhén and John Smellie, Appendix E. They draw a number of general conclusions and remark on the benefit of bringing together hydrogeologists and hydrochemists. Modelling work was assessed by external reviewers and their preliminary conclusions are compiled in appendix F.

5 Task 6 – Performance Assessment Modelling Using Site Characterisation Data (PASC)

This new task was presented by Jan Olof Selroos (Appendix G) and Masahiro Uchida (Appendix H). it was extensively discussed agreed upon to initiate.

The objectives with this task are to:

1. Assess simplifications used in PA models.
2. Assess the constraining power of tracer (and flow) experiments for PA models.
3. Provide input for site characterisation programs from a PA perspective (i.e., provide support for site characterisation program design and execution aimed at delivering needed data for PA).
4. Understand the site-specific flow and transport behaviour at different scales using SC models.

The first objective may be elaborated as follows:

1a. Identify key assumptions needed for long term prediction in PA and identify less important assumptions in PA.

1b. Identify the most significant PA model components of a site.

1c. Prioritise assumptions in PA modelling and demonstrate a rationale for simplifications in PA-models by parallel application of several PA models of varying degree of simplification.

1d. Provide a benchmark for comparison of PA and SC models in terms of PA measures for radionuclide transport at PA temporal and spatial scales.

1e. Establish how to transfer SC models using site characterisation data to PA models, i.e., how to simplify SC models into PA models in a consistent manner.

The specific tasks to be performed are:

Task 6A. Model and reproduce selected TRUE-1 tests with a PA model and/or a SC model. This task provides a common reference platform for all SC-type and PA-type modelling to be carried out as the project progresses. This ensures a common basis for future comparison.

Task 6B. Model selected PA cases at the TRUE-1 site with new PA relevant (long term/base case) boundary conditions and temporal scales. This task serves as a means to understand the differences between the use of SC-type and PA-type models, and the influence of various assumptions made for PA calculations for extrapolation in time.

Task 6C. Develop a 50-100m block scale synthesised structural model using data from the Prototype Repository, TRUE Block Scale, TRUE-1 and FCC. The structural model should also be complemented with a hydraulic parameterisation. It is suggested that a deterministic rather than a stochastic model is constructed so that the differences between models will be results of variations in assumptions, simplifications, and implementation rather than in the structural framework. The structural model will include sufficient elements of the TRUE Block Scale experiment to make it possible to reproduce a TRUE Block Scale tracer experiment as part of Task 6D. It is also suggested that Task 6C is performed by a single group led by SKB in order to provide a structural model that fulfils the needs of all modelling teams.

Task 6D. Task 6D is similar to Task 6A, using the synthetic structural model and a 50 to 100 m scale TRUE-Block Scale tracer experiment. The flow and transport simulations will be carried out using both SC-type and PA-type models. This task provides a common reference platform for all SC-type and PA-type modelling in the considered scale and ensures a common basis for Task 6E.

Task 6E. Task 6E extends the Task 6D transport calculations to a reference set of PA time scales and boundary conditions. In the first part of Task 6E, a basic set of PA and SC assumptions and simplifications should be used. These can be extended to alternative assumptions as part of the sensitivity study part of Task 6E.

Dershowitz presented an example simulation on Task 6, Appendix I.

6 References

Elert M, Svensson H, 2000. Äspö Hard Rock Laboratory. Deconvolution of breakthrough curves from TRUE-1 tracer tests (STT-2) with sorbing tracers. Äspö Task Force, Task 4F.
SKB International Progress Report IPR-00-22.

Elert M, Svensson H. 2000. Äspö Hard Rock Laboratory. Deconvolution of breakthrough curves from TRUE-1 tracer tests (STT-1 and STT-1b) with sorbing tracers. Äspö Task Force, Task 4E.
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SKB International Progress Report IPR-00-16 Part 2.

Shao H, Liedtke L, 2000. Modelling the reactive - radioactive and sorbing tracer tests in fractured rock. Äspö Task Force, Task 4E and 4F.
SKB HRL International Cooperation Report ICR-99-03.

Appendices

TASK 4

A. Modelling of TRUE sorbing tracer tests assuming 3-D flow patterns, Moreno (KTH)

B. T4E&F Evaluation Elert (KEMAKTA)

C. T4F Deconvolution, Elert (KEMAKTA)

D. Overall evaluation, Marschall (Nagra)

TASK 5

E. Summary of results, Rhén (SWECO) & Smellie (Conterra)

F. Review, Bath (Intellisci) & Jackson (AEA Technology)

G. Supplementary Task 5 modeling, Shuttle (Golder) et al

TASK 6

H. Task 6 proposal, Selroos(SKB)

I. Task 6 proposal, Uchida (JNC)

J. Example Task 6 simulation, Dershowitz (Golder)

Appendix A

Task 4

Modelling of TRUE sorbing tracer tests assuming 3-D flow patterns

L Moreno (KTH)

Modelling of sorbing tracer tests assuming 3-D flow patterns

Ivars Neretnieks and Luis Moreno

Chemical Engineering and Technology

Royal Institute of Technology

Outline

- Background
- Aims
- Field data
- Models
- Results
- Conclusions

BACKGROUND

- **Sorbing tracer tests were performed within TRUE-1**
- **Predictions considered Feature A as a 2-D structure**
- **Experimental residence times were longer than predicted/simulated**

AIM

- **To model the Sorbing tracer tests using only field/laboratory data**

FOR SORBING TRACERS

- **FWS/Q determines the interaction with the rock**
- **In our case Q is the extraction rate**
- **What FWS is encountered in TRUE experiment?**

FIELD - LABORATORY DATA

- Sorption coefficients
- Diffusion into matrix
- Rock characterisation to obtain FWS and transmissivity distribution
  - Inflow data in boreholes

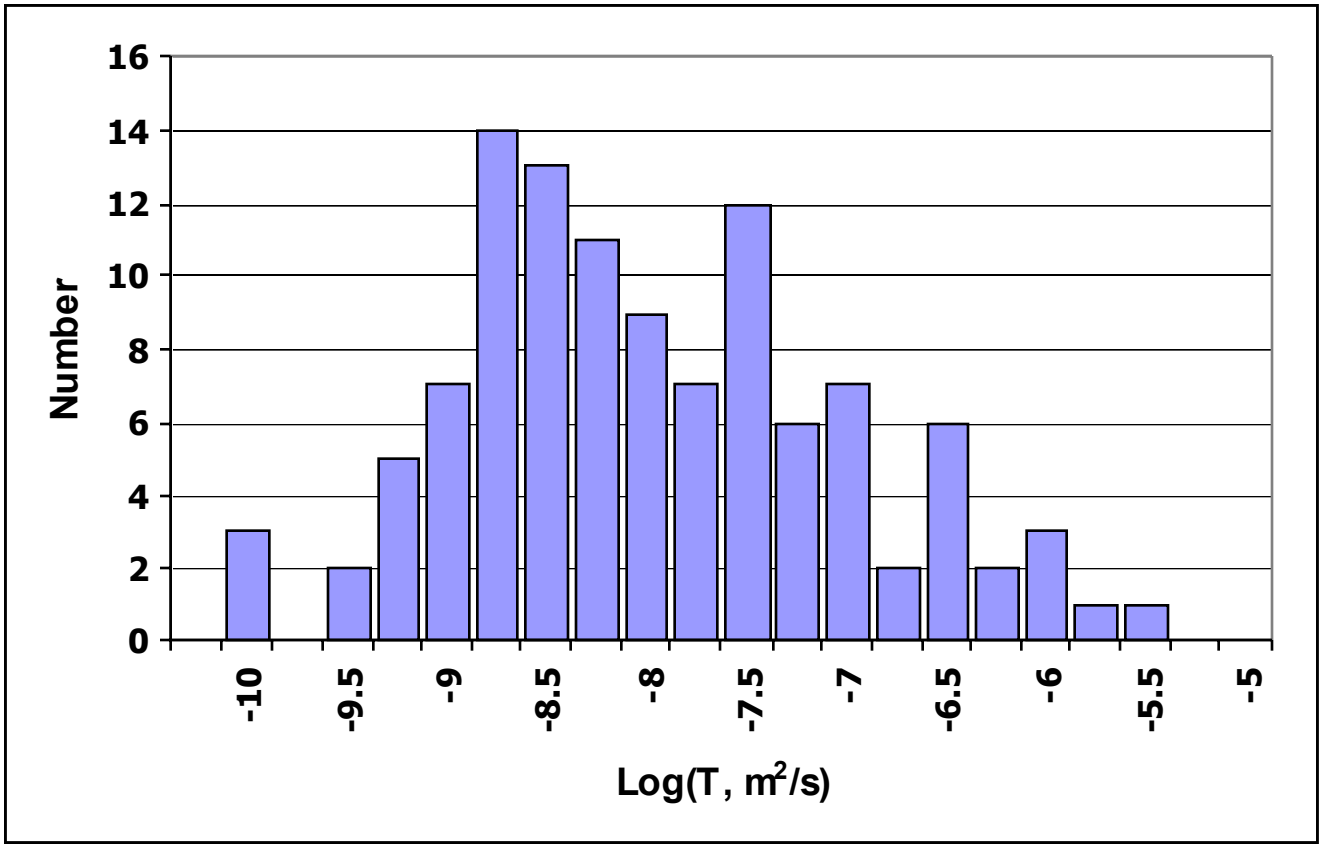
ROCK CHARACTERISATION

- **Data with 0.5 m packer distance**
- **30 % of the sections show inflow below detection level**
- **In average: Boreholes meet one fracture per 0.5 m**
- **Flow wetted surface is estimated to be about 8 - 10 m^2/m^3 rock**

TRANSMISSIVITY DISTRIBUTION

- **Five boreholes: 162, 0.5 m sections in total about 100 m boreholes length**
- **The standard deviation in transmissivity is about 1.00**

INFLOW DATA



INTERFERENCE DATA

- **Cross-hole interference tests show dimensionalities greater than 2.**
- **Connectivity matrix shows connections between Features A and other sections**

MODEL CORE

- **Main effects in all models**
  - **FWS/Q**
  - **De Kd ρ**
- **Secondary effects, all different in different models**
  - **Mixing**
  - **Dispersion**
  - **Network effects**

DETAILS OF MODELS

- **Modelling includes**
  - **Advection in the fracture/channel**
  - **Diffusion into the rock matrix**
  - **Sorption within the matrix**
- **Models**
  - **Multi Channel Model (MChM)**
  - **Channel Network Model (CNM)**
    - » **Code CHAN3D**

IMPORTANT ENTITIES

- **For sorbing species:**
  - **Flow wetted surface (FWS)**
  - **Diffusion coefficient, matrix porosity**
  - **Sorption coefficient**
- **Flow porosity is not important for sorbing species**

MULTI CHANNEL MODEL

- **Simplest of models - captures main effects**
- **Many independent channels**
- **Flow rate in the channels follows a log-normal distribution**

MULTI CHANNEL MODEL

- **Outlet concentration in one channel, e.g., for step input**

$$\frac{c'}{c_o} = \text{Erfc}\left(\frac{LW}{Q}\frac{(D_e K_d \rho)^{0.5}}{\sqrt{t - t_w R_a}}\right)$$

- **For multi channels**

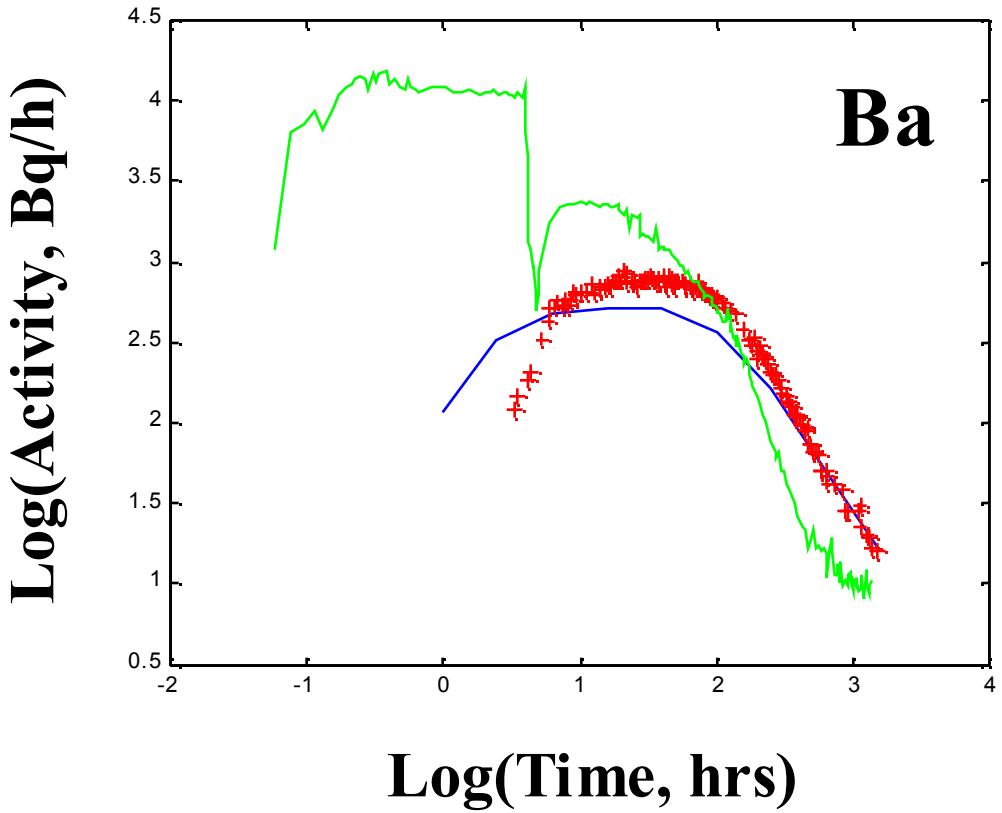
$$\frac{c}{c_o} = \frac{1}{Q}\int_0^\infty q\, f(q)\, c'\, dq$$

USED DATA

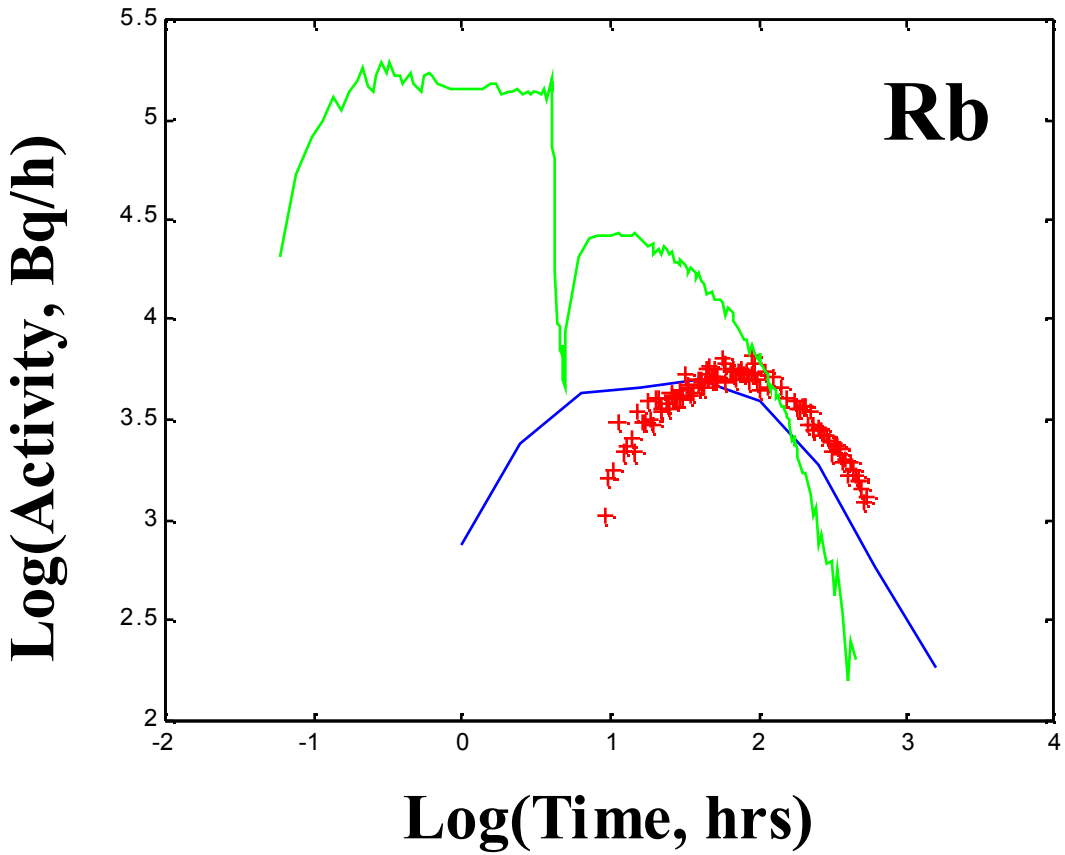
- **Rock data**
  - » **Porosity of matrix = 0.004**
  - » **Rock density = 2700 kg/m^3**
  - » **Pore Diffusivity = 2•10^{-11} m^2/s**

Species	Sorption Constant K_d, m^3/kg	Flow Wetted Surface, m^2/m^3
Ba	0.005	
Cs	0.400	8.0
Rb	0.008	

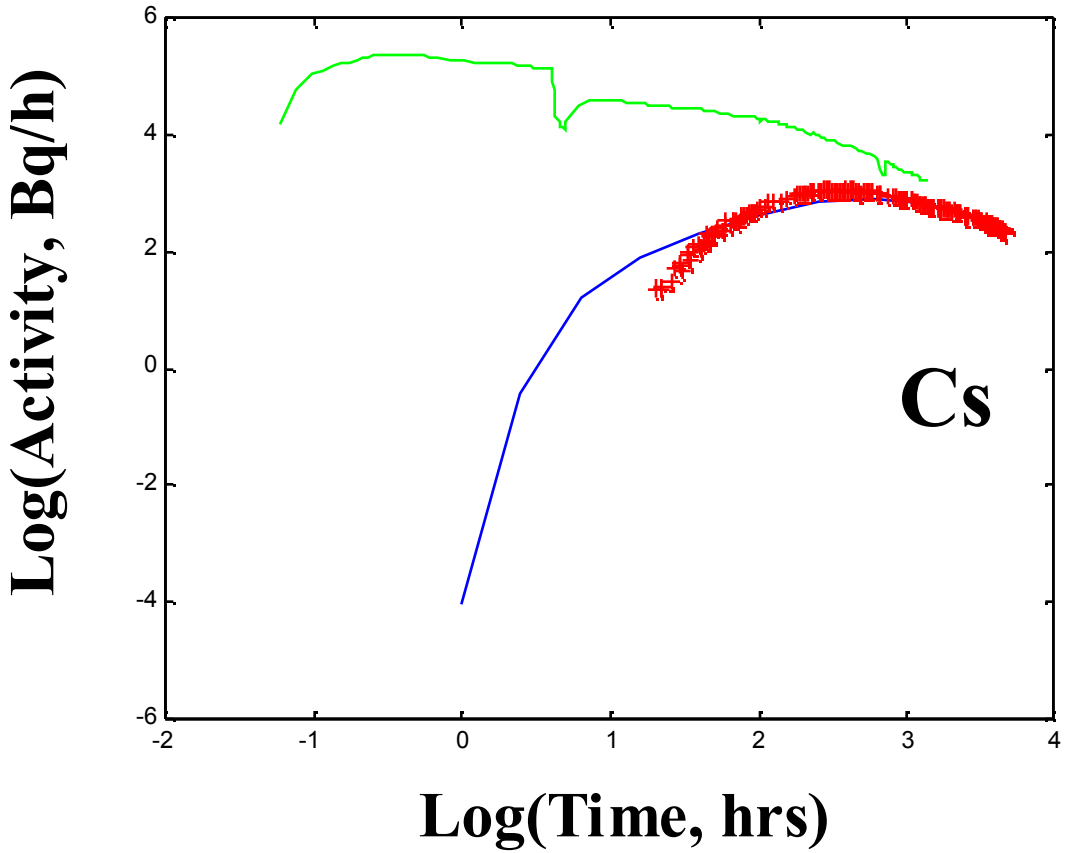
RESULTS - MChM
3-D structure



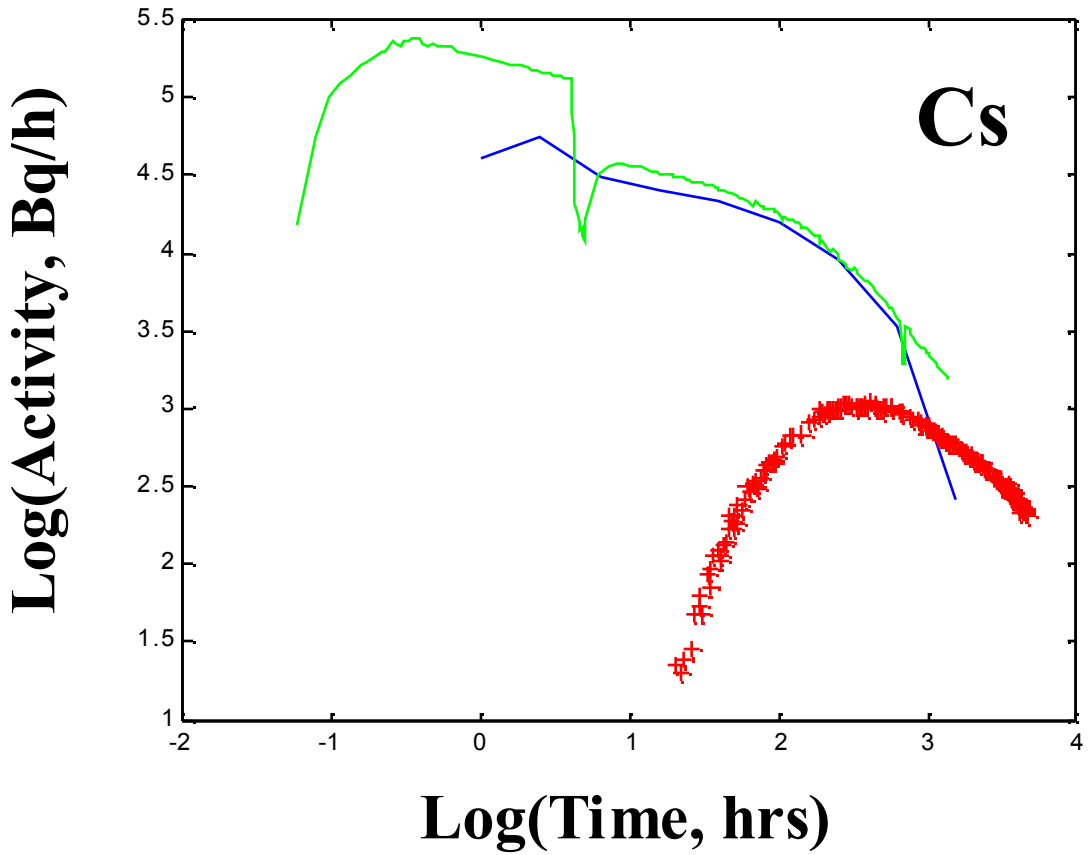
RESULTS - MChM
3-D structure



RESULTS - MChM
3-D structure

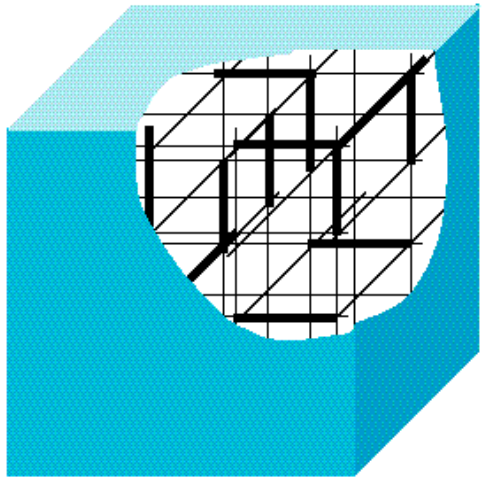


RESULTS - MChM
2-D structure

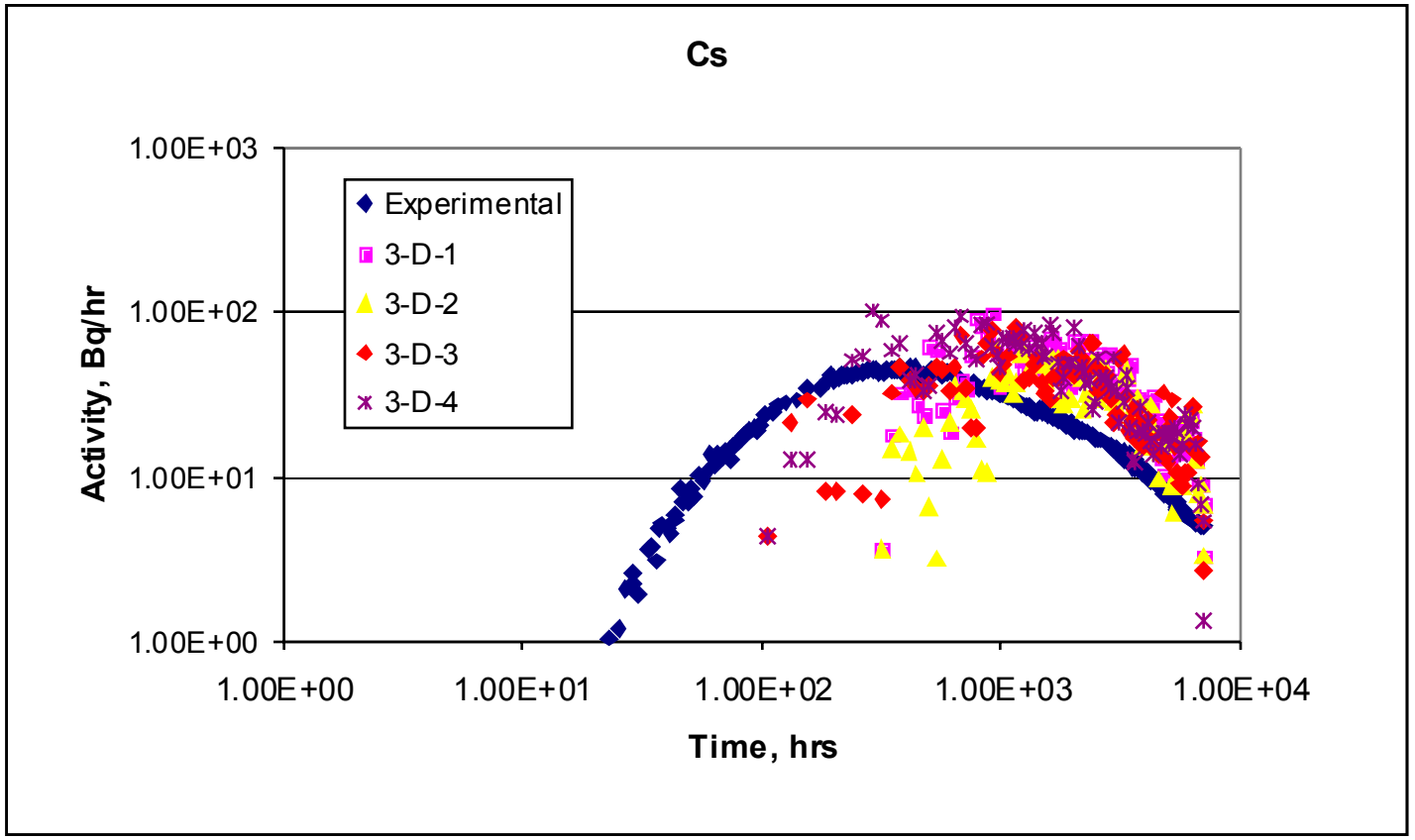


CHANNEL NETWORK

- **Flow through channels**
- **Channels forming a three dimensional network**



RESULTS - CHAN3D
3-D structure



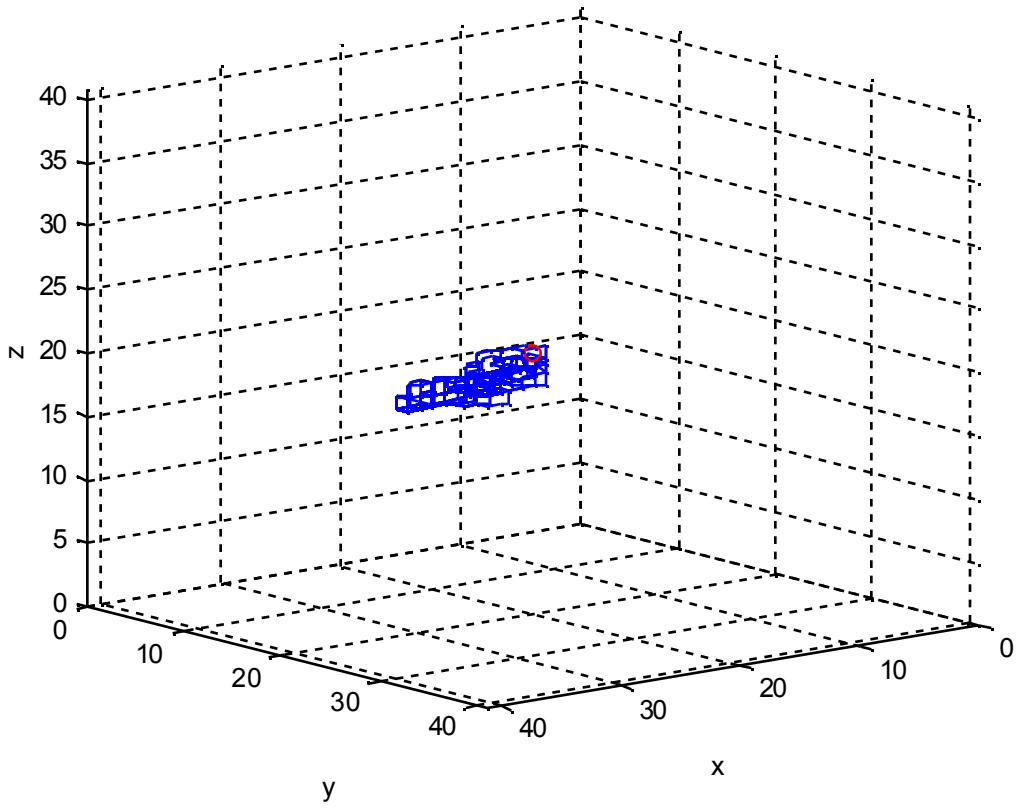
CONCLUSIONS

- **Fairly successful prediction of sorbing tracer RTD using only laboratory and borehole data**
- **No adjustable parameters**

FWS in 2-D and 3-D

$$FWS_{3D} \approx 30\, FWS_{2D}$$

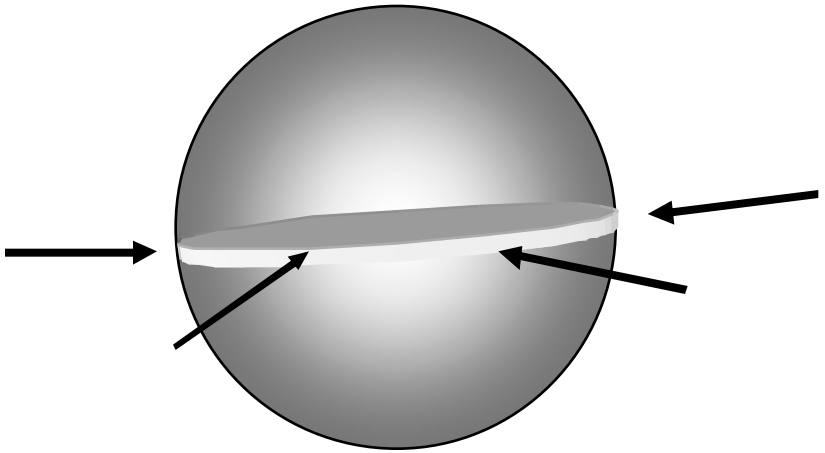
3-D TRACKS

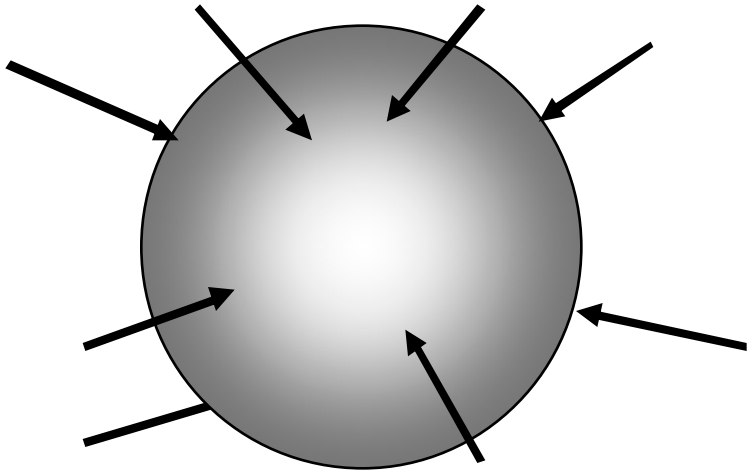


FWS in 2-D and 3-D structures

- FWS in Circle (feature A)= $A_{FetureA}$ $2*\pi r^2=157\ m^2$

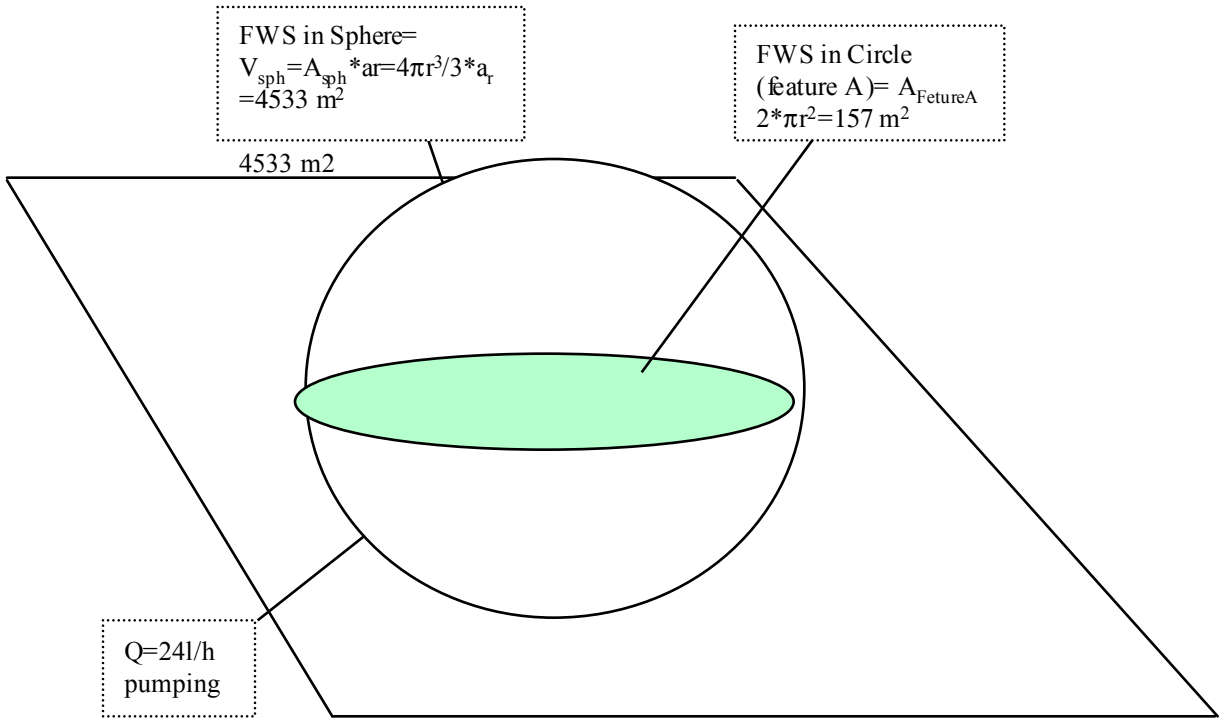
FWS in Sphere= FWS=$V_{sph}*a_r=$ $4\pi r^3/3*a_r=4533\ m^2$





4533/157 = 29

2-D and 3-D FWS


FWS in Sphere=
$V_{sph}=A_{sph}*ar=4\pi r^3/3*a_r$
=4533 m^2
4533 m2
FWS in Circle
(feature A)= $A_{FetureA}$
$2*\pi r^2=157\ m^2$
Q=24l/h
pumping

Appendix B

Task 4E&F Evaluation

M Elert (Kemakta)

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

Äspö Task Force meeting
14-16 November 2000

Mark Elert

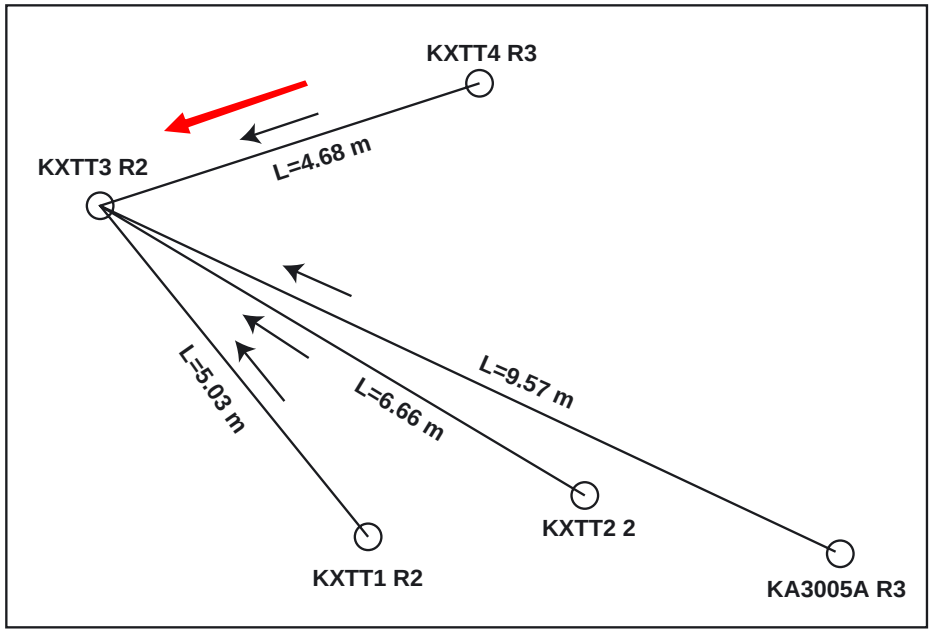
Kemakta Konsult

Introduction

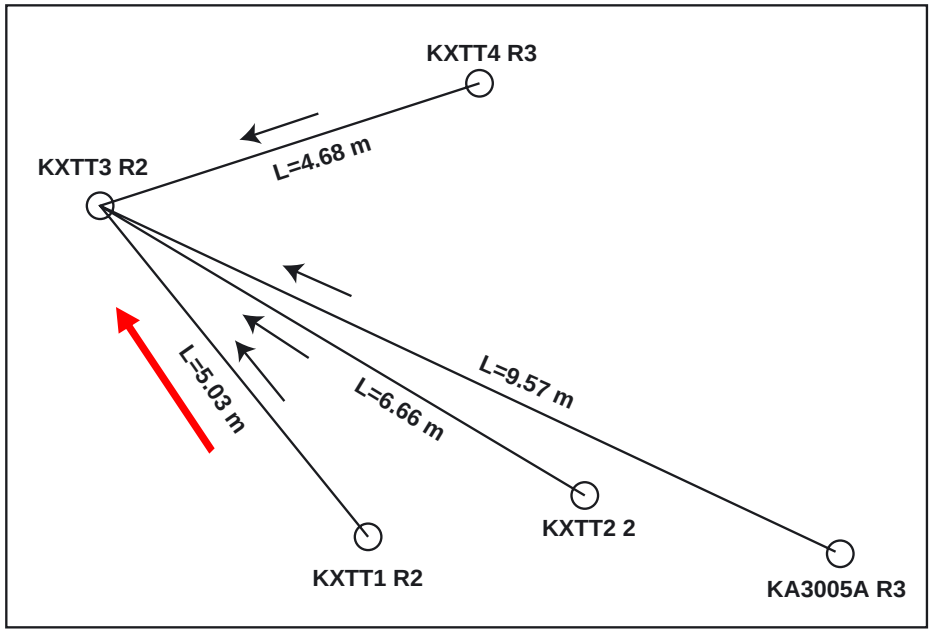
- The evaluation work is ongoing.
  - Final/Draft ICR-reports from modelling groups.
  - Modelling Questionnaires
- Preliminary contents of evaluation report:
  1. Introduction
  2. Purpose and set up of experiment
  3. Modelling approaches
  4. Results
  5. Discussion
  6. Conclusions

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

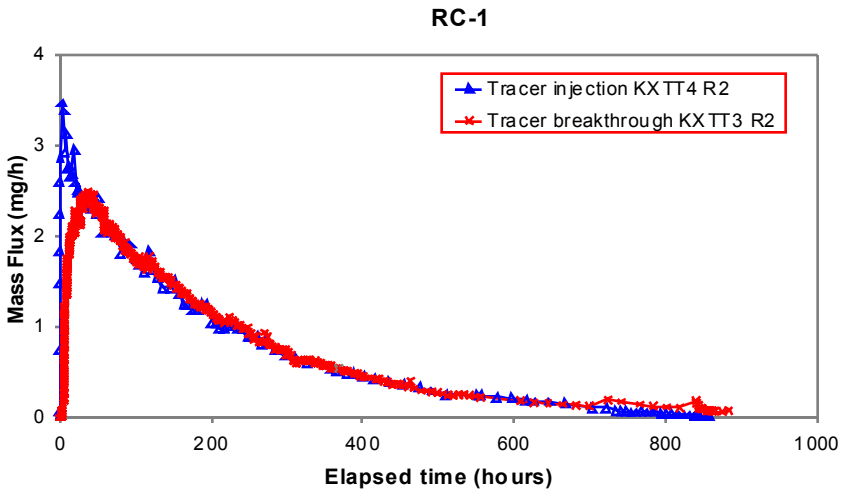
- Types of models
  - Deterministic continuum model (homogeneous/ heterogeneous)
  - Stochastic continuum
  - Deterministic multirate mass transfer model
  - Discrete Fracture Network
  - Channel Network
- Model geometry
  - Most groups considered Feature A as an isolated feature
  - JNC/Golder: Discrete 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

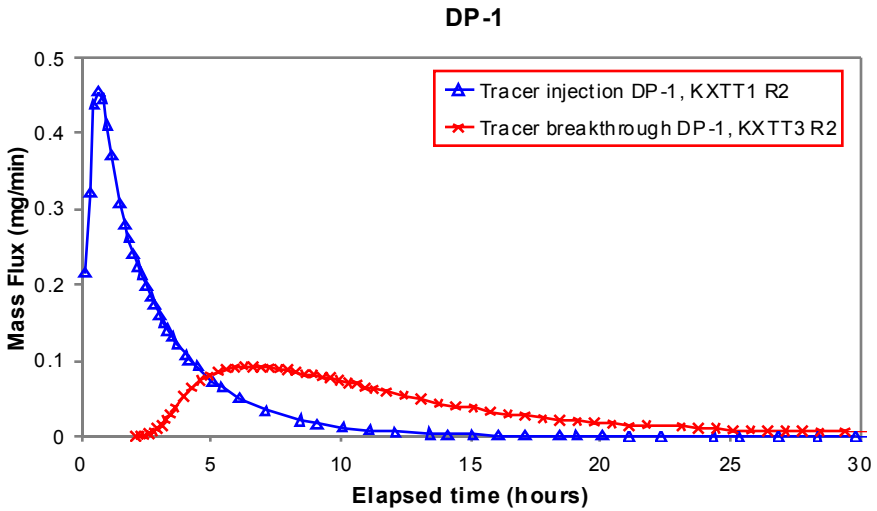
Summary of measured and evaluated parameters for the flow path KXTT4 R3 → KXTT3 R2

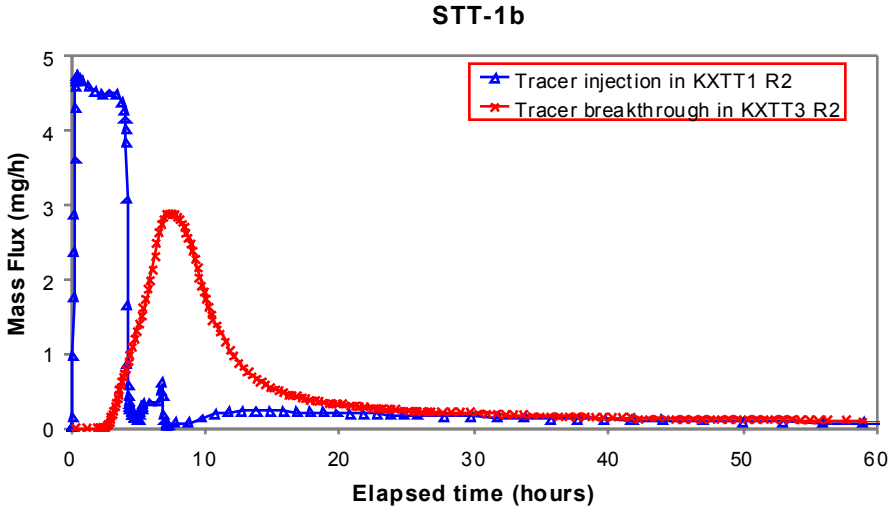
Test*	Q (l/min)	Δh (m)	R (%)	D/v (m)	K_{fr} (m/s)	b (m)	θ_k
RC-1	0.2 (0.4)*	2.8 (6.9)*	100	1.6	$7.1 \cdot 10^{-4}$	$1.4 \cdot 10^{-3}$	$0.5 \cdot 10^{-3}$
DP-5	0.1	3.0	28	0.34	$2.0 \cdot 10^{-4}$	$1.6 \cdot 10^{-3}$	$0.5 \cdot 10^{-3}$
DP-6	0.2	3.6	70	0.48	$4.1 \cdot 10^{-4}$	$2.4 \cdot 10^{-3}$	$0.4 \cdot 10^{-3}$
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***	$1.0 \cdot 10^{-4}$***	$4.5 \cdot 10^{-3}$***	$4.0 \cdot 10^{-3}$***

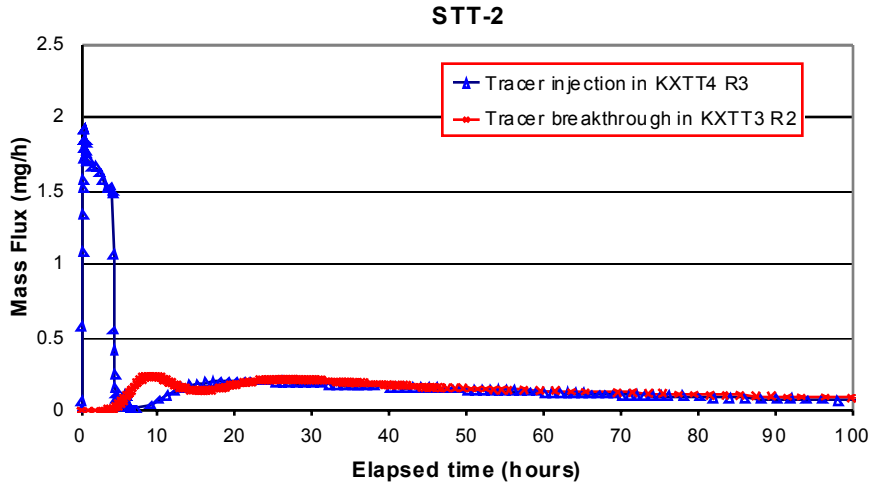
* Pumping increased during experiment
** Flow path #1
*** Flow path #2

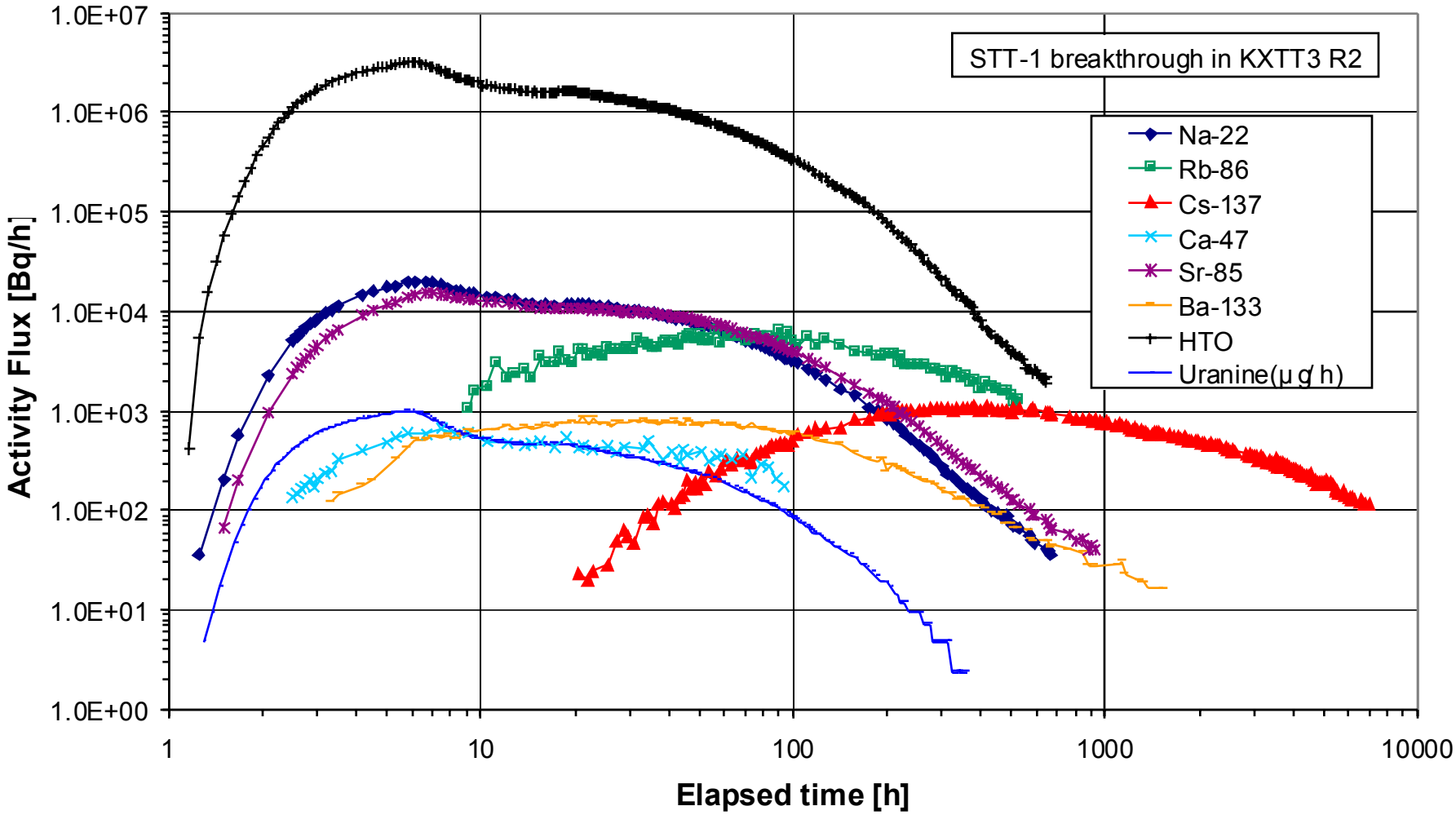
Injection and breakthrough curves



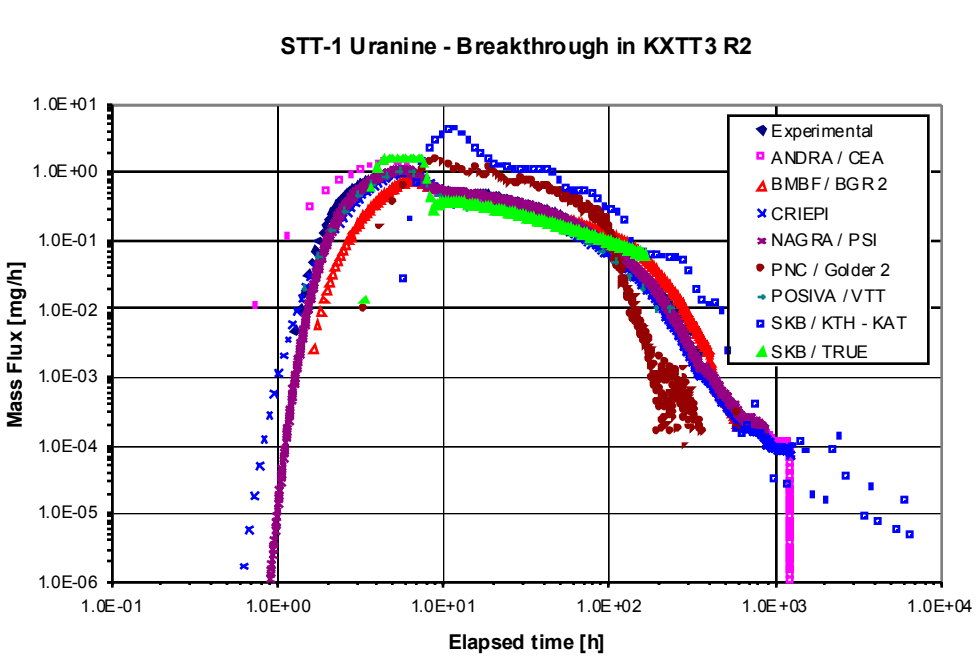


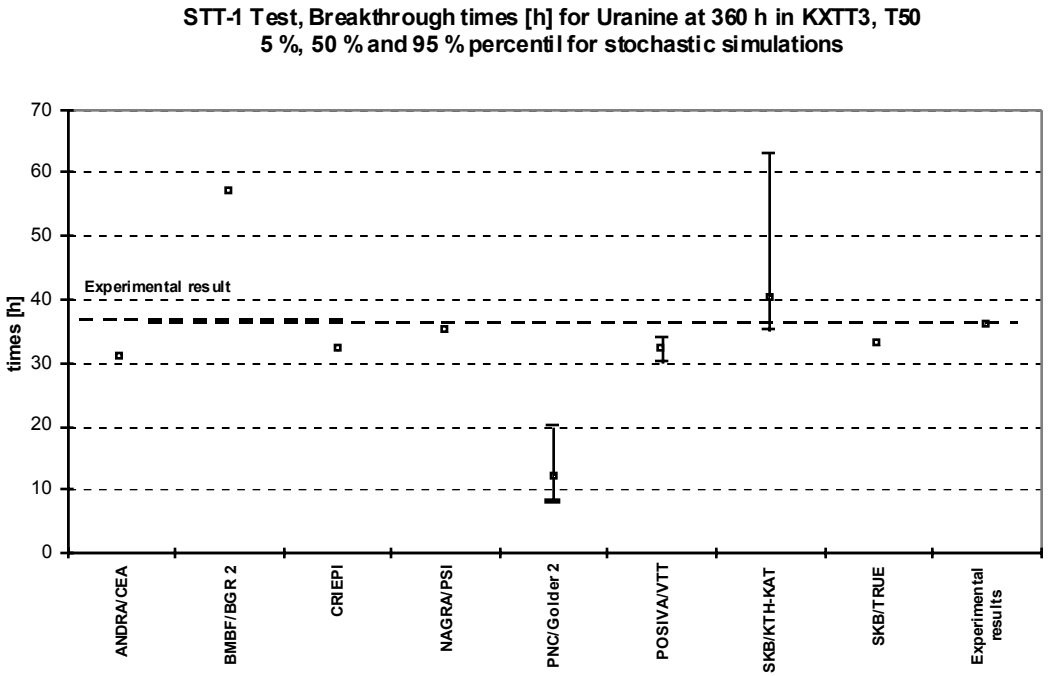





STT-1 breakthrough in KXTT3 R2
Na-22
Rb-86
Cs-137
Ca-47
Sr-85
Ba-133
HTO
Uranine(μg/h)
Activity Flux [Bq/h]
1.0E+07
1.0E+06
1.0E+05
1.0E+04
1.0E+03
1.0E+02
1.0E+01
1.0E+00
1
10
100
1000
10000
Elapsed time [h]

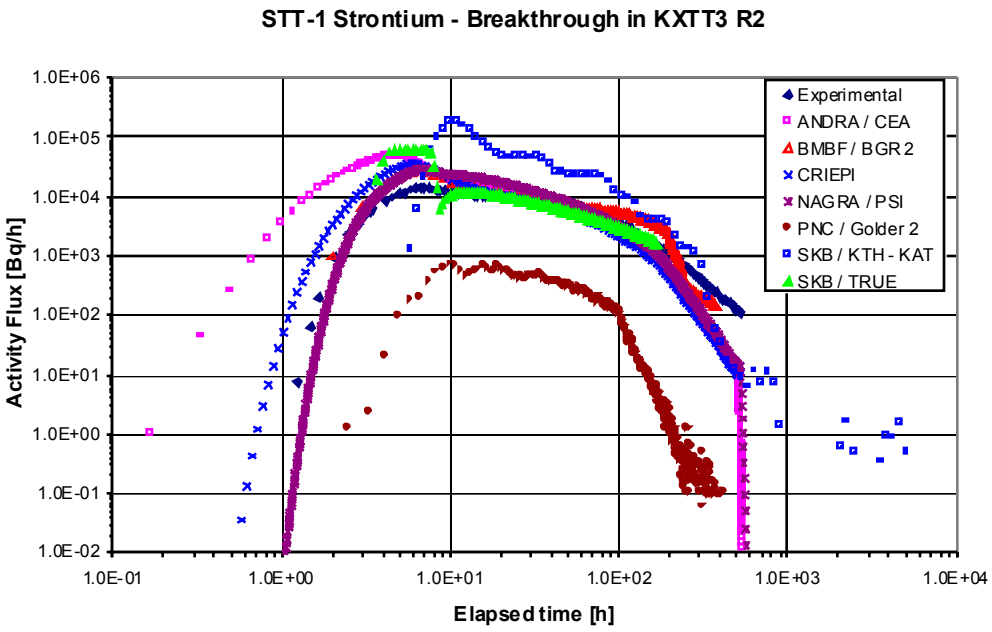
Predictions Uranine STT-1

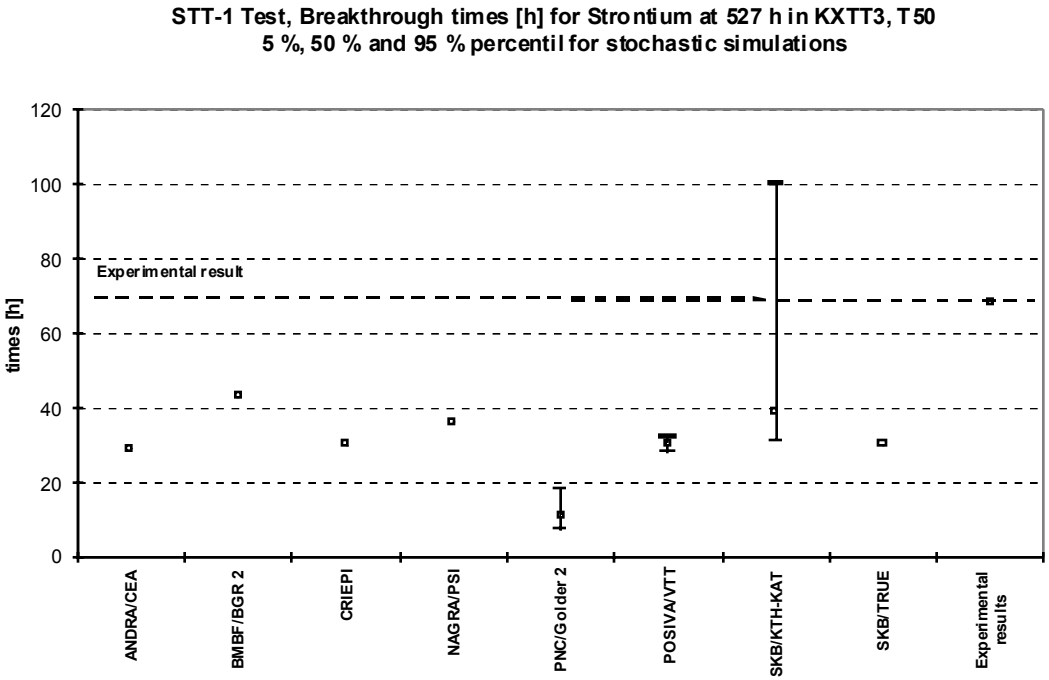




Kemakta

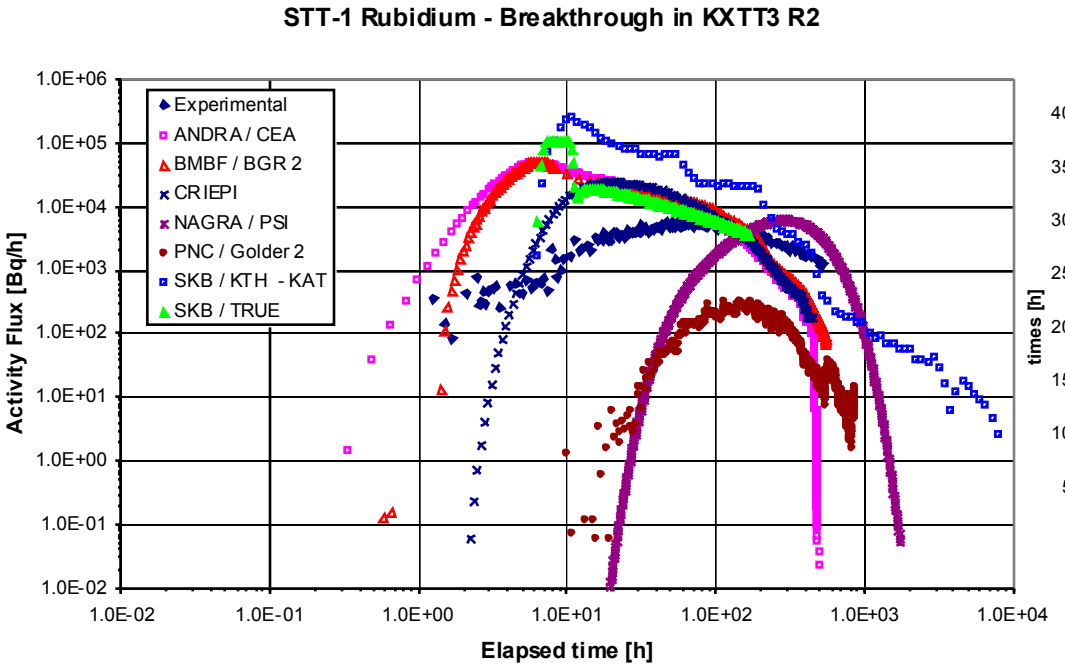
Predictions Sr-85 STT-1

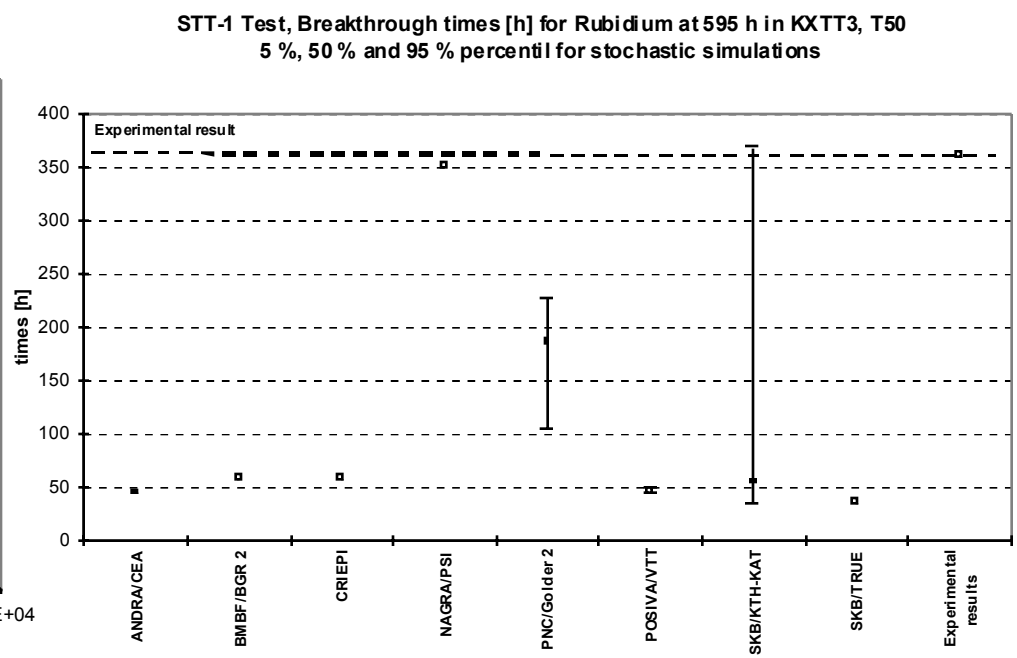




Kemakta

Predictions Rb-86 STT-1

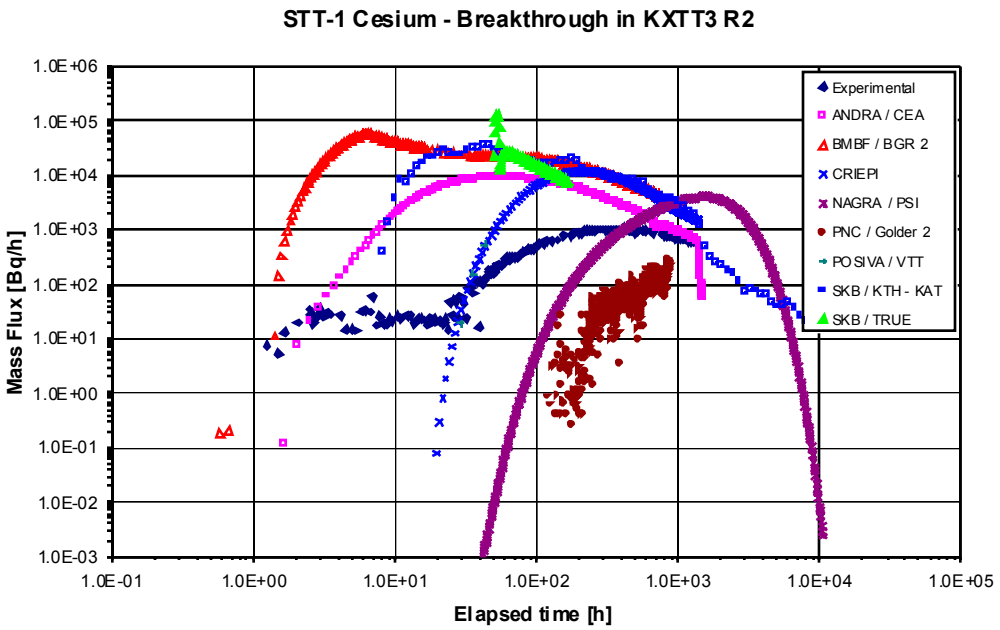


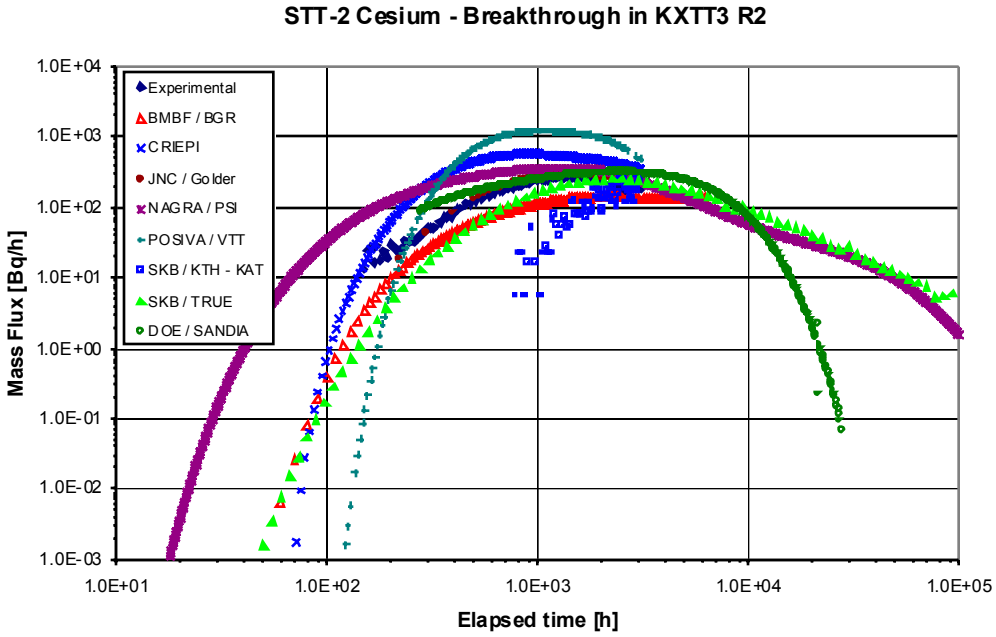


Kemakta

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 sorption 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

Appendix C

Task 4F Deconvolution

M Elert (Kemakta)

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

Äspö Task Force meeting

14-16 November 2000

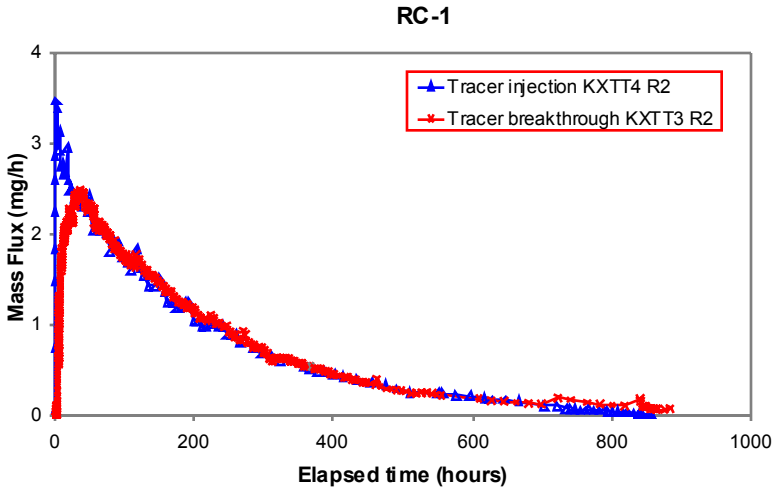
Mark Elert and Håkan Svensson

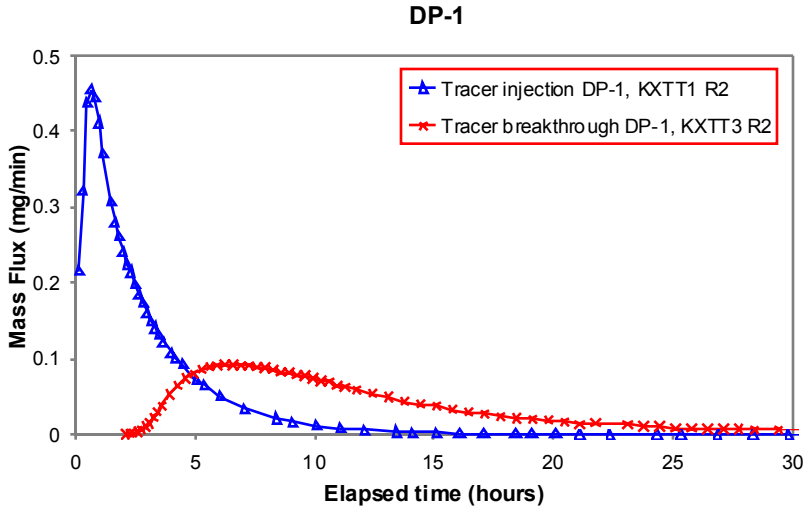
Kemakta Konsult

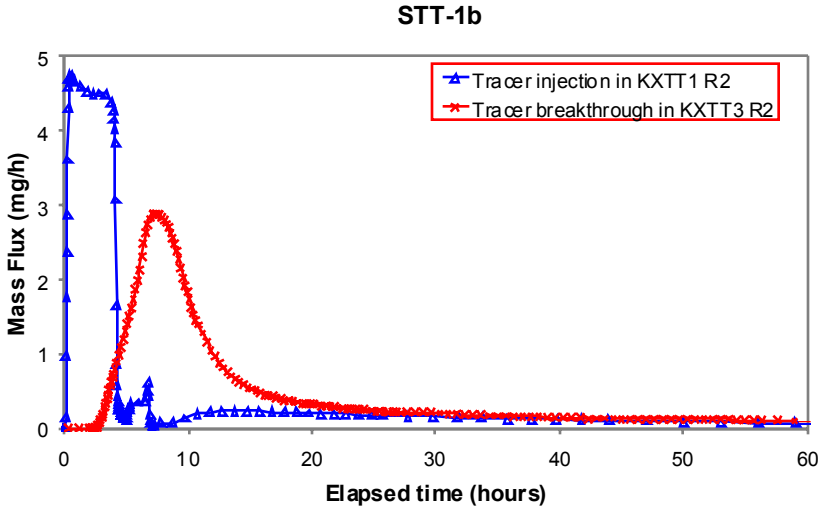
Introduction

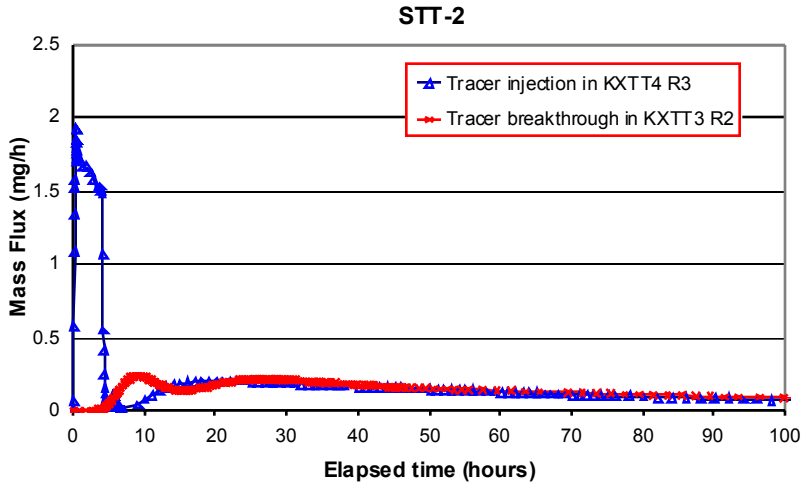
- Short well-defined injection source term beneficial for evaluation of tracer tests
- Proved practically difficult to achieve
- Evolution of injection techniques RC-DP-STT
- Mathematical treatment of experimental data - Deconvolution
  - eliminating the effect of the source term
  - problems with experimental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

Injection and breakthrough curves

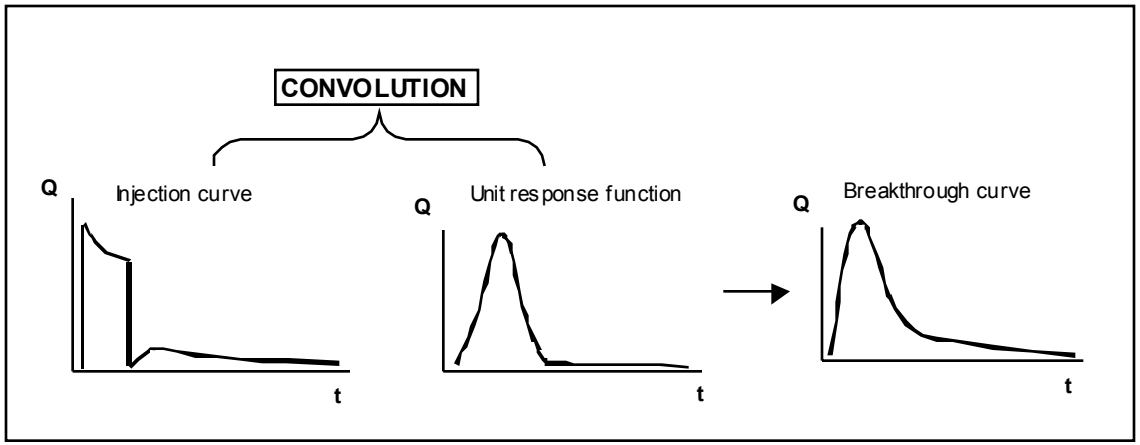








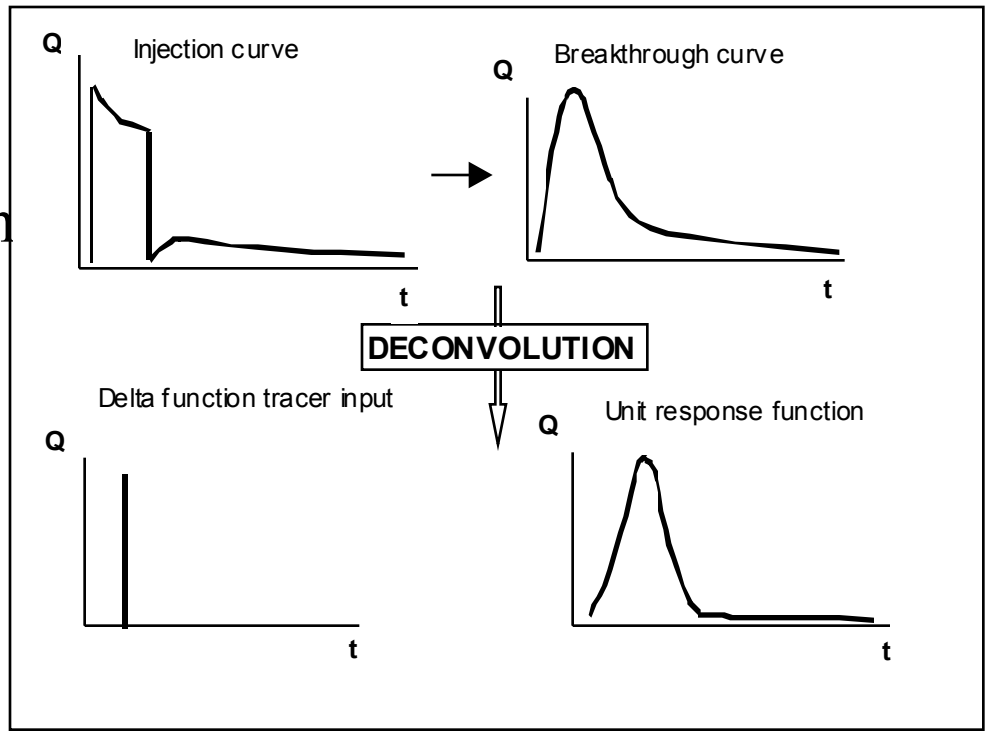
Convolution



- 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.

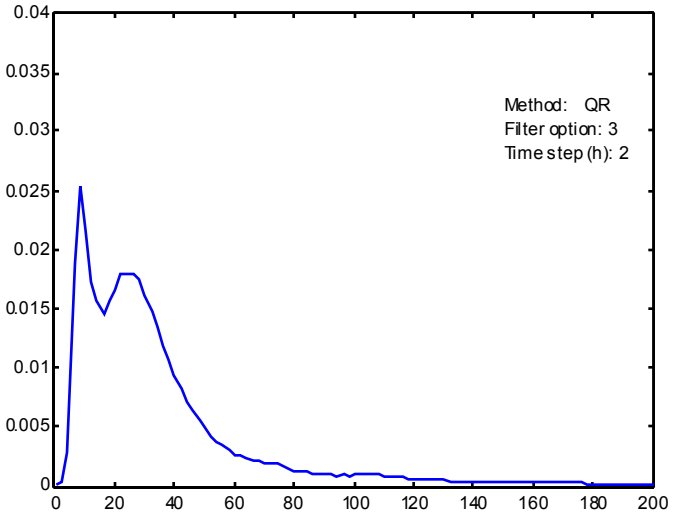
$$M_i = \sum_j a_{ij} \cdot m_j \qquad M_i = \sum_s m_{is} a_s$$

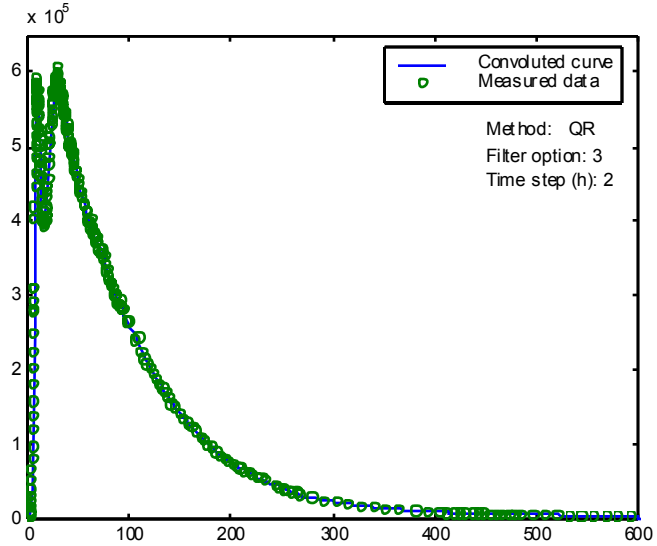
- **M = m•a**
- **a = m^{-1}M**

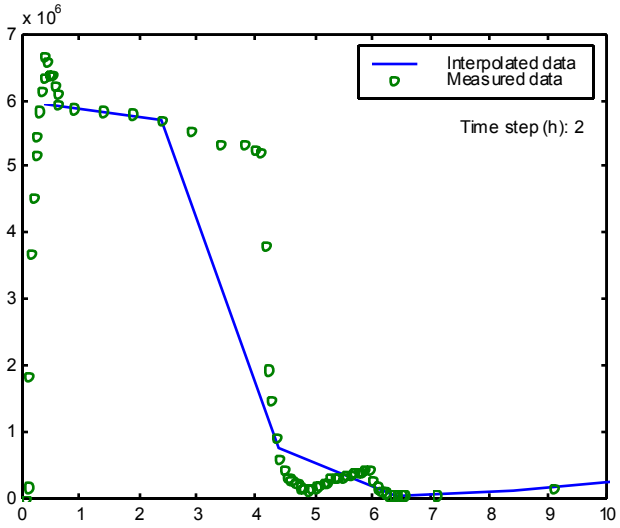
Method used in this study (contd.)

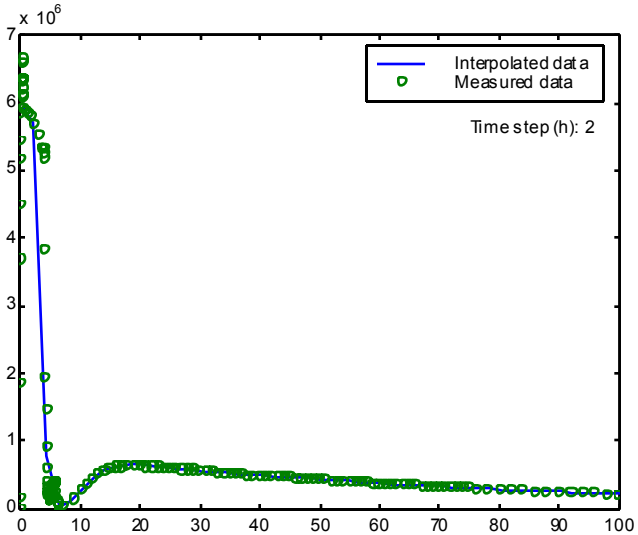
- The Toeplitz method considerably more stable than deconvolution routine of Matlab
- Filtering of breakthrough curves
  - spiky curves were filtered using a moving average filter
  - filter shape and length varied for optimal results
- Convolution of unit response function
  - the result was convoluted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

Deconvolution HTO STT-2

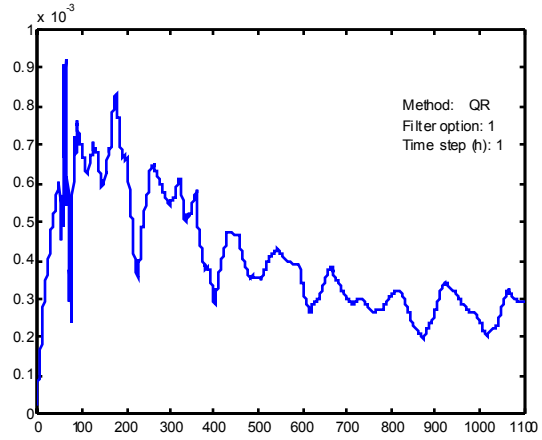


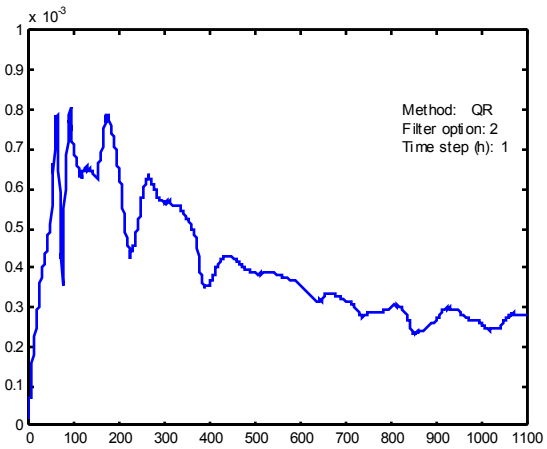


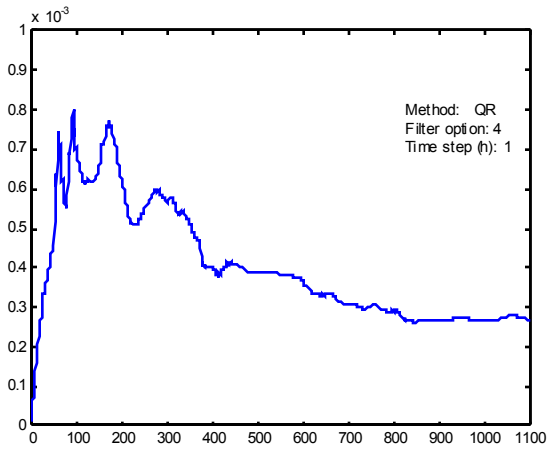


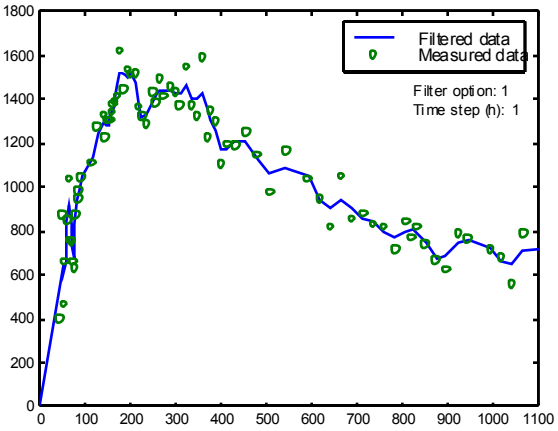


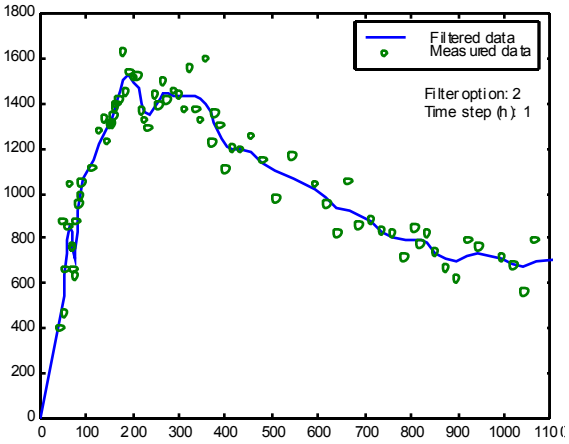
Varying filter length Rb-86 STT-2

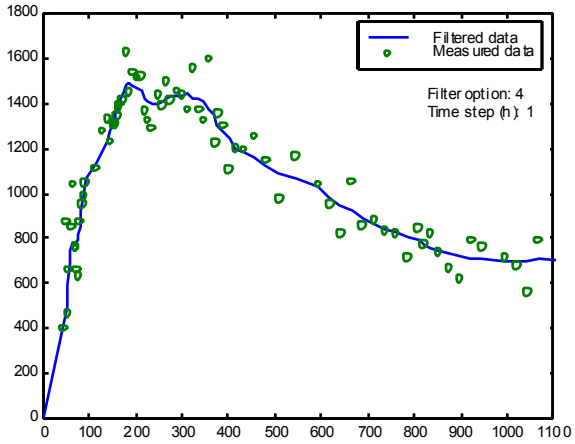




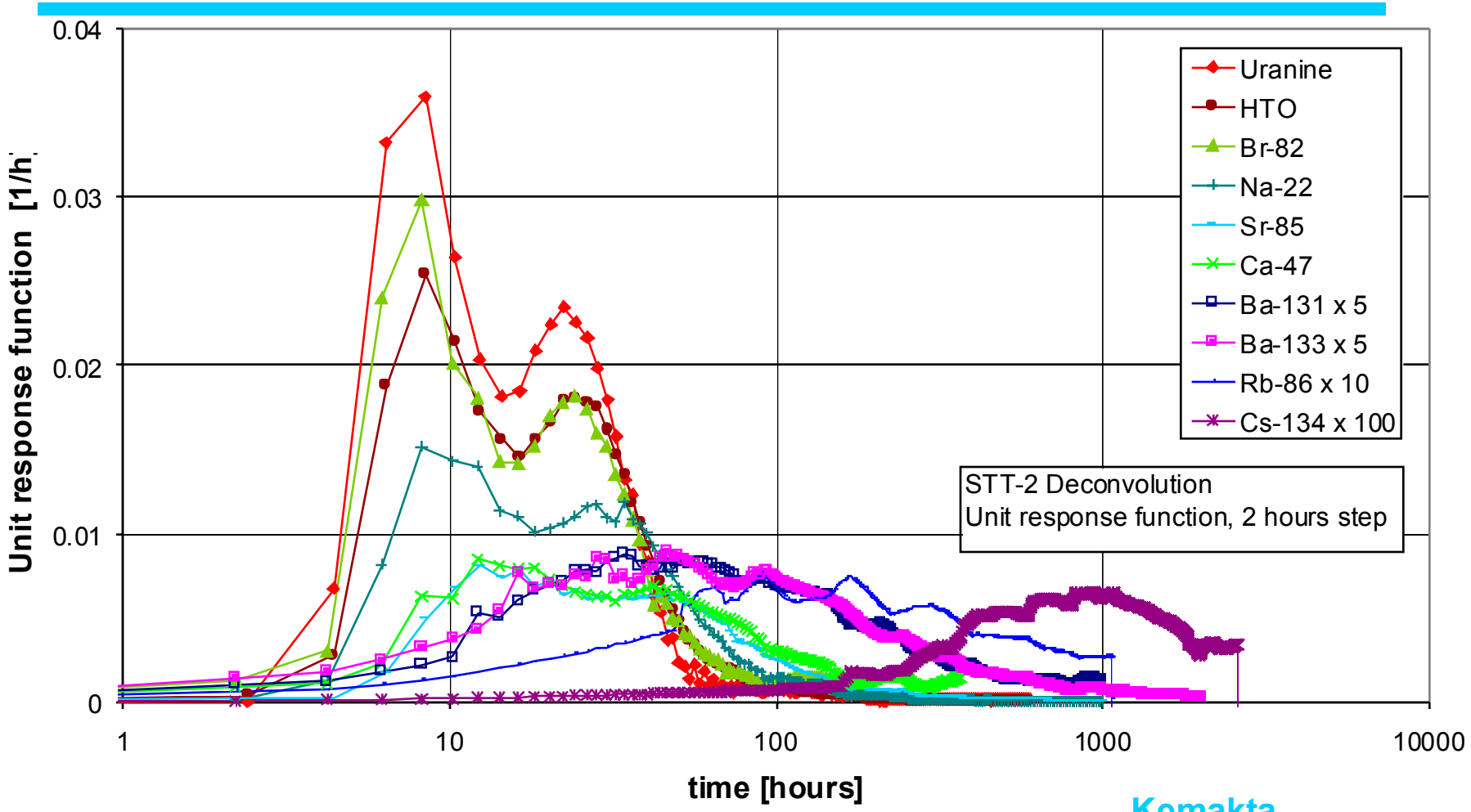








Summary of deconvolution STT-2



Kemakta

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

Appendix D

Task 4
Overall evaluation

P Marschall (Nagra)

Overall evaluation Task 4

- Motivation and Expectations

  ⇒ What did the participating organisations (and their representatives - the **TF delegates**) expect from Task 4?

  ⇒ What did the participating organisations finally learn from Task 4?

  ⇒ Where are the unresolved issues? (**viewpoint of TF delegates**)

Overall evaluation Task 4

- Task overview and expectations
- Task History
- Proposed Evaluation Issues
- Proposed Report Outline
- Milestones and Schedule

Overall evaluation Task 4

- Proposed Evaluation Issues

⇒ What did we learn about solute transport mechanisms?
⇒ Did the modeling task essentially affect tracer test plans (feedback to experiment)?
⇒ Do we have an accepted tracer test interpretation strategy
⇒ Do we have an accepted tracer test interpretation strategy?
⇒ Did performance measures, prediction/evaluation strategies and questionaires work as steering tools?
⇒ Can we proudly present new modelling tools (tool development)?
⇒ Which where the most beneficial SC data for the modellers?
⇒ Which were the most important subtasks in improving process understanding?
⇒ Comparison of conceptual models (flow wetted surface; discrete vs. continuum paths)
⇒ Comparison of evaluation strategies
⇒ Achievements at limited resources; cost / benefits evaluation
⇒ ...

Overall evaluation Task 4

- Proposed Evaluation Issues / Main areas

  ⇒ Understanding of flow and transport processes

  ⇒ Methodologies and strategies in tracer test analysis (and test design)

  ⇒ Steering of future modelling tasks

Overall evaluation Task 4

- Proposed Report Outline

1. Introduction

- Background
- Motivation
- Scope
- Statements by participating organisations

2. Task Overview

- Subtasks and expected output
- Task history (modelling vs. experiment)
- Task concept (reporting, prediction/evaluation, …)

3. Evaluation Issues

- Rationale / Scope
- Highlight selected issues
- …

4. Conclusions and outlook

- lessons learned
- open issues

Overall evaluation Task 4

- Milestones, Schedule and Responsibilities

Overall Evaluation Task 4		
Action	**deadline**	**Resp**
Proposed report outline (extended outline)	end Nov.00	Mlp/ME
Review of report outline	end Dec.00	TF-D, MG
Statements by the participating organisations	end Mar.01	TF-D
Chapters 1-2: Final Draft	Sept. 01	ME/Mlp
Chapter 3: First Draft	June 01	Mlp/ME
Review of chapter 3	Sept. 01	TF-D
Extended outline chapter 4	TF-Meeting	all
…		

Appendix E

Task 5

Summary of results

I Rhén (SWECO)
J Smellie (Conterra)

Task 5: Project scope and objectives (PR HRL 98-07)

- The aim of Task 5 is to compare and ultimately integrate hydrochemistry and hydrogeology.
- The general method is to compare the outcome of an independent hydrochemical model with an independent groundwater flow model.
- Data from the pre-investigation and construction phases of Äspö HRL is used.
- Objectives:
  - To 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
  - To develop a procedure for integration of hydrological and hydrochemical information which could be used for disposal site assessments.

Task 5: Rationale

- Groundwater flow and chemistry are important for conditions for the safety and performance assessment of a deep geological disposal of radioactive waste.
- If groundwater flow and chemistry are integrated properly it should give better confidence in the description of the present and future conditions at a site.
- The modelling approach(es) used in Task 5 considered successful could be used for any future repository site investigations and evolution, especially in a crystalline bedrock environment.

Task 5: Data sets provided (1)

- 1 Hydrochemical data 1
- 2 Hydrogeological data 1
- 3 Hydrogeological data 2
- 4 Hydrochemical data 2
- 5 Geographic data 1
- 6 Hydro tests and tracer tests
- 7 Hydrochemical data 3, update of data delivery 4 based on new end-members. Recommended to be used instead of 4.
- 8 Performance measures and reporting 1
- 9 Hydrogeological data 3

Task 5: Data sets provided (2)

- 10 Geographic data 2
- 11 Boundary and initial conditions
- 12 Performance measures and reporting 2
- 13 Transport parameters compiled
- 14 Hydrochemical data 4
- 15 Co-ordinates for the test sections defining the control points
- 16 Co-ordinates for bore holes drilled from the tunnel
- 17 Hydrogeological data - prediction period
- 18 Hydrochemical data - prediction period.

Task 5: Data provided since Task Force meeting 13 (1)

- Structure of I data deliveries requested according to the performance measures.
  - Results (Exel files):
    - Particle traces to cp:s
    - Mixing proportions at cp:s (calculated and measured)
    - Conservative tracers at cp:s (calculated and measured)
    - Piezometric head (calculated and measured)
    - Water table
    - Sinks and sources for Na, K, Ca, Mg, SO_4, HCO_3 (mg/L)
  - Questionnaire (Word file)
  - Final report , including flow chart showing the modelling/evaluation steps (Word file and paper copy)

Task 5: Data provided since Task Force meeting 13 (2)

- Structure of digital data deliveries
  - General: Delivered as EXEL files
  - Water table and particle traces to cp:s in the Äspö co-ordinate system (unit: m) for tunnel positions 1400, 2100, 3000, 3600m.
    - (format description)
  - Preferred format for **time series**
    - (format description)

Task 5: Data provided since Task Force meeting 13 (3)

- Structure of digital data deliveries:
  - General: Delivered as **EXEL files**
  - **Water table and particle traces** to cp:s in the Äspö co-ordinate system (unit: m) for tunnel positions 1400, 2100, 3000, 3600m.
    - Observation point, Secup, Seclow, CP No., Time. (Preferred file name: Ptrace_xxxx_yyyy, where xxxx is the tunnel face position (for example 1400) and yyyy is the organisation name (for example JNC)
      - Row 1 in data file: Observation point, Secup, Seclow, CP No., Time.
      - x,y,z, (in columns, x positive: directed to the EAST)
    - Water table, Time . (Preferred file name: Watertable_xxxx_yyyy, where xxxx is the tunnel face position (for example 1400) and yyyy is the organisation name (for example JNC)
      - Row 1 in data file: Water table, Time .
      - x,y,z , (in columns, x positive: directed to the EAST)

Task 5: Data provided since Task Force meeting 13 (4)

- Structure of digital data deliveries:
  - Preferred format for **time series**
    - Data in columns:
      - Observation point, Secup, Seclow, CP No., Time (modelling time in days), Date (YYYY-MM-DD), result1, result 2, ……
    - Mixing ratios in the order: **Brine, Glacial, Meteoric, Baltic Sea**
    - Calulated values for at least **every month**, and start time and stop time according to performance measures (1990-10-01 to at least 1997-01-01)
    - Deliver **predictions** and the **re-modelling** according to the above format
    - Deliver **all pressures** coupled to an observation point (=**bore hole section**) (calculated and measured, side by side, ….date, P(calc), P(meas))

Task 5. List of model approaches used by each group

Organisation	Flow modell	Mixing calc.	Reaction modelling
ANDRA-ANTEA	HCD(c)+HRD(c, double porosity), (MHFE)	x	
ANDRA-CEA	HCD(c), d, (MHFE)	x	
ANDRA-ITASCA	HCD(c), (FE)	x	x
BMWi	HCD(c), (FE)	x	x
CRIEPI	HCD(c)+HRD(c), (FE)	x	x
ENRESA	HCD(c), (FE)	x	x
JNC	HCD(c)+HRD(DFN), (FE)	x	
POSIVA	HCD(c, double porosity)+HRD(c, double porosity), (FE)	x	x
SKB	1:HCD(c)+HRD(sc), 2: HCD(c)+HRD(DFN⇒c), (FDM)	x	x

HCD: Hydraulic Conductor Domains, HRD: Hydraulic Conductor Domains, d: density driv. flow
c: Continuum, sc: Stochastic continuum, DFN: Discrete Fracture Network

Task 5: Hydrochemical Modelling

Undisturbed hydrochemical conditions: Pre-excavation stage

- Involves water-rock interaction processes and the mixing of groundwaters from different origins.
- The greater the groundwater flow-rate through the bedrock the greater the likelihood that mixing processes dominate.
- Under natural conditions Äspö, at least down to 500-600 m, represents a hydrodynamically active system. For example, flow due to hydraulic gradients, water level fluctuations and earth-tidal effects may cause some mixing.
- The question is whether the total system can be modelled using a near-equilibrium geochemical approach?

Task 5: Hydrochemical Modelling

Disturbed hydrochemical conditions: post-excavation stage

- Activation of additional mixing processes
- May have also disturbed the thermodynamic equilibrium thus stimulating chemical reactions
- Some of the chemical reactions may be biologically mediated
- Additional mixing processes and chemical reactions can have a significant impact on modifying the local groundwater chemistry

Task 5: Hydrochemical Modelling

The M3 model:

- M3 (***M***ultivariate ***M***ixing ***M***ass balance calculations) was developed to mathematically and objectively classify different groundwater types on the basis of chemistry and degrees of mixing and reactions.
- By identifying the major groundwater sources, i.e. reference water end-members, each groundwater sample can be described by a mixture of all or some of these reference waters by summarising the chemical information in a Principal Component Analysis plot.
- M3, since it considers the effects from mass balance reactions, also has the added advantage of indicating when water/rock interactions are important.
- M3 uncertainties: end-members, sampling, analytical, conceptual, methodology. Stated uncertainty of the method is +/- 0.1 mixing units and detection limit uncertainty is <10% of a mixing portion.

Task 5: Hydrochemical Modelling

The M3 Model

Selected end-members:

- Meteoric water - precipitation from the 1960s and infiltration
- Baltic Seawater - modern seawater from Baltic sea
- Brine (saline) water - deep (1700 m) water from Laxemar
- Glacial water - meltwater from last glaciation (10 ka ago)

Based on:

- detailed hydrogeochemical study of the Äspö site
- detailed palaeohydrogeological study of the Äspö site
- comparison with other Fennoscandian sites

Task 5: Hydrochemical Modelling

M3 modelling approach:

- Mixing portions of the selected end-member reference groundwaters are calculated for each sampled location.
- If there is agreement between the calculated and measured values, elemental behaviour can be explained by an ideal mixing model.
- Mass balance reactions are used to define sources and sinks for different non-conservative elements which deviate from the ideal mixing model used in the mixing calculations. Deviation indicates potential chemical reactions.
- Integrated use of the geochemical equilibrium PHREEQE code can relate these sinks and sources to active chemical processes.

Task 5: Hydrochemical Modelling

Influence of chemical reactions

SKB identified the following reactions as being potentially important:

- *Organic decomposition* in the uppermost part of the bedrock - can result in a gain of HCO_3 in the system
- *Organic redox reactions* in the shallow part of the bedrock - can result in a gain of Fe and HCO_3 in the system
- *Inorganic redox reactions* in the shallow part of the bedrock - can result in a gain of SO_4 in the system

Task 5: Hydrochemical Modelling

- *Dissolution and precipitation of calcite* - can result in a loss or a gain of Ca and CO_3
- *Ion-exchange* particularly in the presence of fracture clay material - can result in a change in Na/Ca ratio
- *Sulphate reduction* by microbiological activity in the upper bedrock - can result in a loss of SO_4 and a gain of HCO_3

Task 5: Hydrochemical Modelling

SKB; M3 modelling strategy

- Calculate the mixing proportions and chemical changes in the groundwater chemistry at selected Control Points due to tunnel construction
  - Make predictions for Control Points, initially up to tunnel position 2900 m
  - Make predictions for Control Points, subsequently from tunnel position 2900 to 3600 m
- Compare the outcome of the predictions at all Control Points with the measured values
- Compare the results of the chemical mixing and reaction modelling with the hydrodynamic modelling data

Task 5: Hydrochemical Modelling

SKB; M3 Results:

- M3 predictions show a general agreement with the measured values at the Control Points.
- Major deviations from ideal mixing are shown by Na^{+}, Ca^{2+}, HCO_3^{-} and SO_4^{2-}, which is consistent with other hydrochemical studies made at Äspö.
- M3 can be used for predictive purposes if there is a time series of observations - this is the case for short-term predictions (years to tens of years).
- For long-term predictions (hundreds of years), M3 calculations should be guided by the hydrodynamic model.

Task 5: Hydrochemical Modelling

Modelling approach of BMWi

- Deviations from an ideal mixing model can be identified by applying a chemical model.
- The hydrogeochemical model used is based on PHREEQC (Version 2) which can handle speciation, batch reaction and inverse geochemical calculations.
- The model indicates:

  - which processes dominate and to what extent

  - which constituents and pure phases participate in the reactions

Task 5: Hydrochemical Modelling

BMWi input data:

- Measured time series groundwater chemistry was used to to simulate compositions at the Control Points
- Most important ions used: Na^+, Ca^{2+}, Mg^{2+}, Cl^-, HCO_3^-, SO_4^{2-},
- Most important reactions considered:
  - Dissolution/precipitation of carbonate
  - Dissolution/precipitation of gypsum
  - Dissolution/precipitation of $Mn(OH)_2$
  - Carbonate chemistry
  - Sulphate chemistry

Task 5: Hydrochemical Modelling

BMWi; Calculations and results:

- For each water sample the proportions of the different groundwater end-members were calculated using chloride, sodium and ^{18}O as conservative tracers
- Using these proportions the non-conservative elements were determined
- These non-conservative elements showed a deviation from the measured values
- This deviation was minimised by equilibrium calculations
- Due to the revised mixture ratios the concentrations of the non-conservative species, i.e. Ca^{2+}, Mg^{2+}, HCO_3^-, SO_4^{2-} (exception K^+), are in better accordance with the measured values. Reactions are significant!

Task 5: Hydrochemical Modelling

Modelling approach of CRIEPI:

- Initial compositions of the four recommended end-members were first defined, based on the measured chemistry
- The chemical species of the mixed water (i.e. at the Control Points) were then calculated from the mixing proportions as predicted from the M3 results
- This was repeated using the mixing proportions as predicted from the FEGM/FERM results
- Finally, these mixed water compositions were modelled using the geochemical equilibrium HARPHRQ code to identify which major geochemical reactions have contributed to the calculated chemistry

Task 5: Hydrochemical Modelling

CRIEPI; Most important reactions considered:

- HCO_3 production - decomposition of organic material
- Consumption of dissolved oxygen - pyrite oxidation
- Dissolution and precipitation of calcite
- Cation exchange by clay minerals
- Oxidation/reduction between HS^- and SO_4^{2-}

Task 5: Hydrochemical Modelling

CRIEPI; Results:

- decomposition of organic material appears to control the concentration of HCO_3^- in the majority of cases
- cation-exchange reactions are significant
- taking both reactions into consideration resulted in a closer agreement with the measured values

Task 5: Simulation of M3 End-member Mixing Ratios

General statement:

- All modelling groups participated in this simulation exercise
- These mixing ratio simulations provided the first means to integrate hydrochemistry and hydrogeology - only one group attempted a coupled reactive transport model.
- Regardless as to the reliability or otherwise of the M3 mixing ratio calculations, the use of a common database was critical in allowing comparison between the different groups
- In some cases a full and direct comparison between groups was not possible due to different levels of ambition, achievement, available time and resources and model development

Task 5: Simulation of M3 End-member Mixing Ratios.

Approach of ENRESA/Univ. La Coruna:

- Good agreement was obtained between the results computed by the hydrodynamic groundwater flow and solute transport numerical model, and the results of the M3 mixing model
- Comparison between the hydrodynamic model and M3 mixing ratios requires care due to the uncertainties in the mixing model and interpolations
- Initial concentration field is the most important source of uncertainty

Task 5: Simulation of M3 End-member Mixing Ratios.

Approach of SKB:

- Calculated M3 mixing ratios have been reproduced by independent hydrodynamic modelling thus underlining the fact that mixing proportions can be used to compare/integrate/support hydrodynamic models.
- The hydrodynamic model predicts an evolution of the groundwater composition during the construction phase of the Äspö tunnel which is in fair agreement with the mixing portion calculations based on field data, in terms of averages and trends.
- Boundary conditions have a significant effect on the results (vertical boundaries).
- Problems with the long-term storage of Glacial water indicate modification of the conceptual model.
- Variability in the flow-field : a question of comparison with measured data.

Task 5: Simulation of M3 End-member Mixing Ratios.

Approach of JNC:

- Phase 1: Hydrogeological modelling - only head calibration
- Phase 2: Hydrochemical calibration - mixing proportion at Control Points (Glacial component in particular)
- Changes due to hydrochemical input:
  - problems to find significant glacial reserves - added structure to connect with the north of Äspö island
  - modified boundary conditions on Äspö island to constant flux due to the Meteoric water input
  - Baltic sea water input: introduced Baltic sea skin and increased flow porosity

Task 5: Alternative End-member Mixing Ratios

Posiva; Background:

- An alternative method of calculating end-member mixing ratios was carried out by Posiva.
- The method is based on an inverse-modelling approach which is a combination of speciation modelling and mole balance modelling
- Providing constraints on the method is the speciation modelling, petrographic observations, reactions expected to dominate in the groundwater system, and groundwater isotopic data.
- The computations are handled by the PHREEQC-2 program
- Since different groundwater end-members are used, plus different criteria employed in calculating the mixing ratios, this approach cannot be compared directly with the M3 calculations and therefore forms a separate study within Task 5.

Task 5: Alternative End-member Mixing Ratios

Posiva; Input data:

From palaeohydrogeological considerations a total of seven reference groundwaters have been identified which correspond to four, hydrogeochemically significant stages: Present, Litorina, Glacial and Preglacial. The reference groundwaters selected are:

- Meteoric
- Seawater
- Postglacial (seawater that has infiltrated bottom sea sediments)
- Litorina Sea (7 500-7 000 BP)
- Glacial Melt (Pleistocene)
- Preglacial Altered (deduced from Quaternary history)
- Saline (most saline sample at Äspö)

Task 5: Alternative End-member Mixing Ratios

Posiva; Calculation procedure:

- Basically, inverse modelling describes the chemical evolution of groundwater by giving exact estimates of the mixing and geochemical reactions among known initial water compositions needed for reaching a known final water composition
- The pre-investigation dataset (undisturbed) was used to identify the reference groundwater types that have been active at Äspö
- The tunnel impact dataset (disturbed) was used to monitor the effects of construction on the groundwater chemistry
- The calculations are carried out in steps, assuming steady-state chemical reactions

Task 5: Alternative End-member Mixing Ratios

- ***Posiva;***
  - The calculations are based on the assumption that Cl and ^{18}O behave conservatively
  - All other chemical values used in the calculations are subject to mole transfers - i.e. they are involved in dissolution/precipitation to/from reacting phases to satisfy the calculation constraints
  - The directions of dissolution/precipitation reactions will move towards achieving steady-state conditions
  - A previously successful step (assuming steady-state) will lead to the next step
  - These steps ultimately extend to the reference waters, and then to the mixing fractions

Task 5: Alternative End-member Mixing Ratios

Posiva: Conclusions:

- Results show three extensive sources of groundwater that attempt to intrude into the Äspö site during open tunnel conditions
- These reference groundwater types are: meteoric water, fresh Baltic Seawater and saline groundwater.
- Geochemical reactions related to these types are strong (Baltic), moderate (meteoric) and weak (saline).
- The inverse model approach, unlike the M3 approach, is not mathematically based. However, model testing (not within Task#5) using similar end-members resulted in agreement between the two approaches.
- Consequently, in terms of globally interpreting the hydrochemical data for the Äspö site, both methods are in general accordance.

Task 5: Coupling of Transport and Geochemistry

Approach of ANDRA/Itasca:

- How can geochemistry help to improve the reliability of the hydrodynamic modelling?
- What kind of complexities can be expected by the simultaneous coupling of geochemistry and hydrodynamics?

Task 5: Coupling of Transport and Geochemistry

ANDRA/Itasca; Hydrodynamic Modelling:

- Discrete Fracture Network Model type was used, allowing for channeling within fracture planes by the use of one-dimensional pipes
- The transport model was first calibrated based on groundwater flow computations, and then calibrated using the geochemical data (e.g. Chloride)
- Mixing ratios at the Control Points were used to calibrate the skin factor at the bottom of the Baltic sea
- The use of hydrochemical data significantly decreased the uncertainty of the simulations

Task 5: Coupling of Transport and Geochemistry

ANDRA/Itasca; Coupling with geochemistry:

- Fully coupled reactive transport modelling was restricted to part of the model domain
- Modelling approach assumes thermodynamic equilibrium - reaction kinetics are considered either very fast or very slow with respect to the groundwater residence times
- Chemical species were preferred to the M3 mixing ratios. The principal components (i.e. initial conditions) selected were: Na^{+}, Ca^{2+}, CO_3^{2-}, Cl^{-}, SO_4^{2-}, Mg^{2+} and K^{+}.

Task 5: Coupling of Transport and Geochemistry

- ***ANDRA/Itasca;***
- The major reaction of concern selected was calcite dissolution/precipitation
- This reaction type was extended to include to magnesium carbonates and gypsum
- All relevant soluble chemical complexes to this problem were included using the CHEMVAL database

Task 5: Coupling of Transport and Geochemistry

ANDRA/Itasca; Simulations:

- Coupled transport modelling was used to simulate the impact of tunnel construction over a period of 100 days
- Simulations indicate that variable water salinity influences the aqueous solution ionic strength and consequently the 'apparent' chemical reaction constants
- Reactive transport results show that even in zones where geochemistry is considered as simple and of little importance, (e.g. in the absence of significant redox or surface reactions), transport of chemical species might in fact be affected by mineral precipitation/dissolution, therefore constraining the hydrodynamic modelling

Task 5: The use of chemical data- Summary

Integration of hydrogeological and hydrochemical modelling

- simple simulation of mixing ratios (+/- chemical reactions) to calibrate (consistency check) the hydrogeological model
- hydrochemical time series data at CPs can reflect changes in the hydrodynamic flow conditions
- use of salinity (density) data to simulate large-scale hydrodynamic flow conditions
- coupled flow and multicomponent reactive transport modelling

Task 5. General Conclusions

Groundwater mixing proportions

- Results essentially validate M3 as being a useful semi-quantitative tool to calculate mixing proportions and to present and interpret hydrochemical data.
- Posiva's mixing proportion calculations using different end-members also provides a good alternative approach.

Integration of hydrodynamic and hydrochemical modelling approaches

- A comprehensive comparison between groups has not been possible due to different levels of ambition, achievement, available time and resources, and model development

Task 5. General Conclusions

- ***Hydrodynamic modelling***
- Most groups were successful in calibrating and testing their respective models to simulate aspects of the Äspö groundwater flow conditions.
- Chemistry, in the form of single species or M3 mixing ratios, was used mainly to calibrate and modify parameters and structures.

Task 5. General Conclusions

Hydrochemical Modelling

- Hydrochemical modelling was attempted by 70% of the groups.
- All groups treated the groundwater mixing ratios in the hydrodynamic simulations as conservative, i.e. assuming no water/rock reactions.
- Hydrochemical reaction modelling, assuming thermodynamic equilibrium conditions, was carried out by several groups. Generally, this was successful and showed that reactions have some effect on the groundwater chemistry and therefore the calculated groundwater mixing ratios.
- However, geochemical reactions, whilst significant, are largely overshadowed when compared to mixing processes.

Task 5. General Conclusions

Coupled transport modelling

- Fully coupled reactive transport modelling, albeit restricted, was carried out by one group.
- Modelling of Redox Zone: Successful integration of hydrodynamics and chemical reactions, but not representative of the Äspö site as a whole.

Task 5. Final Comment

- Task 5 has been successful in bringing together two scientific groups who traditionally have viewed each other with mutual suspicion
- Hopefully the hydrogeologists have learned to see groundwater, not as a commodity to be pumped or injected here and there, but as a means of supporting (or otherwise) the validity and consistency of their models by understanding its chemistry
- Hopefully the hydrochemists have learned that they no longer can hide behind volumes of analyses and multiple hypotheses; the time has come to put their ideas to the test and see if they stand up to a more rigorous examination

Task 5: Status of reporting

Status of TASK 5 - Final reporting, 2000-11-13								
Organisation			**Delivered: x or date**					
						Result files		
	Draft report		**Final report**		**Que.**	**PeM.**		**Comments**
						Phase 1	**Phase 2**	
	(pc)	**(d)**	**(pc)**	**(d)**	**(d)**	**(d)**	**(d)**	
ANDRA / ANTEA	,000703	,000703				,000703		Corr. sent 001024.Will update after Task 14 meeting
ANDRA / CEA			,000531	,000907	,000907	,991216		Should update content list and app.Update Que.
ANDRA / ITASCA			,000727	,000727	,991218	,000727		Update Que.?
BGR / BMWi	-	,000208			,000714	,000125		
CRIEPI		,000411			,001106	,001106		Digital data del. also 00-10-25. Time for final report?
ENRESA / UDC			,000201	,000201	,000201	,000711		Titel page updated. May come a new version
JNC / GOLDER	-	991222				991216		2 or 3 reports?
POSIVA / VTT				,001011	,001011	,001011		Exec sum recieved 001110
SKB / CFE / Intera			,001113	,001112	,001112	,000124		Not all parts of report delivered
pc=paper copy								
d= digital								
Que.=Questionnaire								
PeM.=Perf. Measures								

Task 5: Status of reporting

- Amount of requested data for Performance measures over-ambitious ?
- Limit new requests to mixing proportions at control points for model1 (predictions) and model 2 (with all data available)?
- New request: properties (transmissivity and transport aperture (porosity-width)) for the HCD (large fracture zones) and how they have developed after each modelling step?

Task 5: Status of reporting

- Final Reports latest December 2000
- Questionnaire latest December 2000
- Deliveries (December 2000) - if not already delivered digitally or included in Final Reports:
  - mixing ratios at Control Points (initial conditions - modelling Phase 1 & 2 time series)
  - parameter changes due to calibration (initial conditions - modelling Phase 1 & 2):
    - Properties of HCD (transmissivity, flow porosity - width)
    - Upper boundary conditions on land (flux; head)
- Paper copies of Final Reports to reviewers by February 2001
- Printed versions by Spring 2001
- Draft of Summary and Review Reports by June 2001

Appendix F

Task 5 Review

Adrian Bath (Intellisci)
C Peter Jackson (AEA Technology)

Aspo Task 5 Review

Adrian Bath [+] and C Peter Jackson [*]

[+] Intellisci

[*] AEA Technology

Introduction

- Task 5 objectives
- Summary of activities
- Model acceptability
- M3 issues

Introduction (continued)

- Calibration issues
- Confidence-building issues
- Other issues
- Have the objectives been met?
- Recommendations

Task 5 Objectives

- To 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
- To develop a procedure for integration of hydrological and hydrochemical information which could be used for disposal site assessments

Numerical Models

- Eleven participants with different models and approaches – 9 flow/transport models plus 2 geochemical/mixing inverse models
- Flow modelling methods
  - fracture network, pipe network, dual porosity
  - deterministic fractures ± permeable matrix
  - particle tracking for flow paths and travel times
- Geochemical models
  - mixing and mass balance models
  - reaction modelling coupled with flow & mass transport

Numerical Models

Characteristics of models for Aspo Task #5

	CEA/DMT	ITASCA	ANTEA	GOLDER	CRIEPI	BGR	SKB	VTT	ENRESA
Hydraulic conductor domains	X	X	X	X	X	X	X	X	X
Internal variabiity within HCDs						X		X	
Rock mass domains			X	X	X		X	X	
Sea-bed 'skin'		X		X			X		
Tunnel grouting	X								
Extra features		X		X					
Dual porosity			(X)						
Variable density	X				X		X		
Freshwater	X	X	X	X		X		X	X
Finite difference							X		
Finite element	X		X		X	X		X	X
2D fractures		X		X		X		X	X
Grid fitting	X	X	X					X	
Fracture smearing					X		X		
Fracture network				X					
Channel network		X		X					

Boundary Conditions

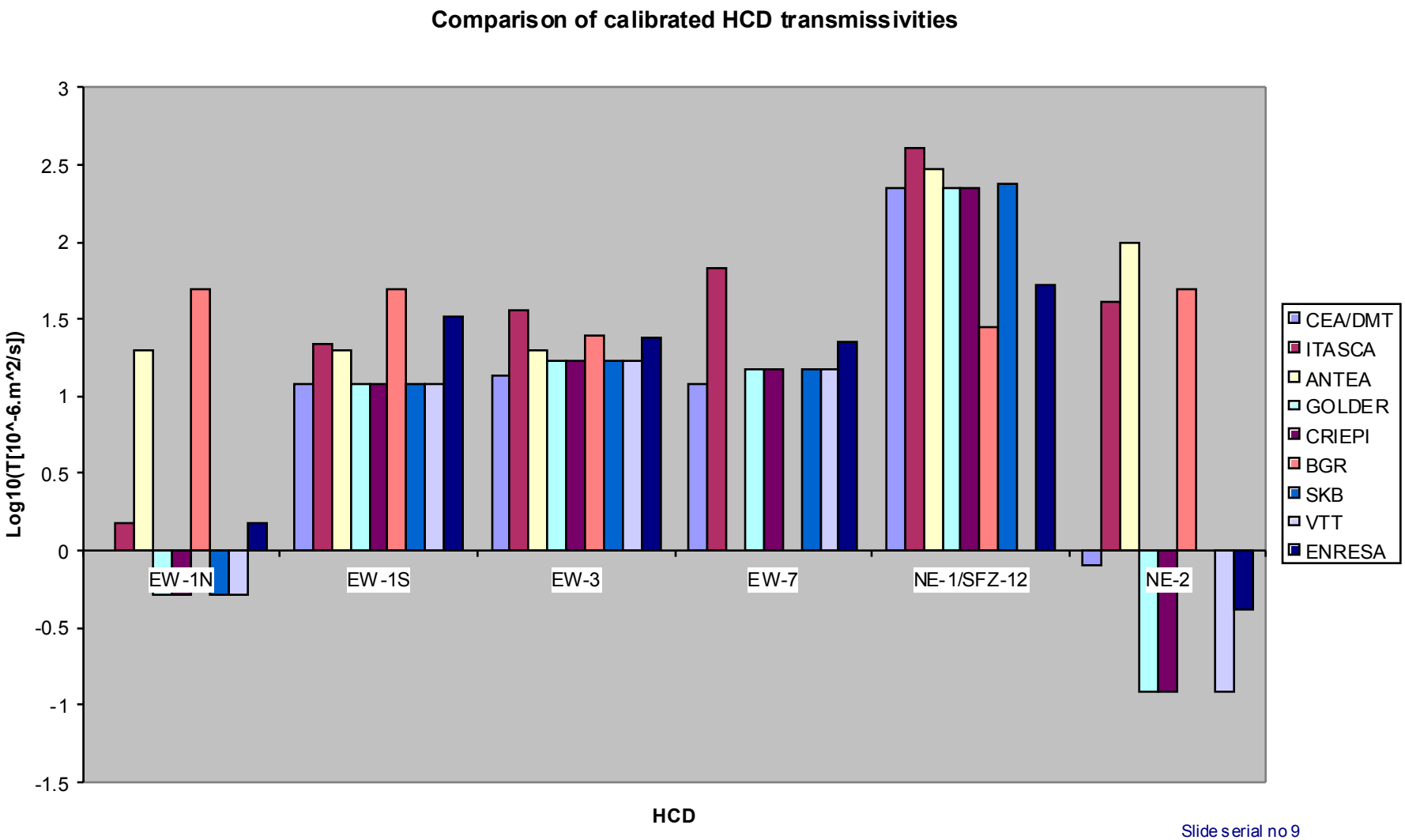
Boundary conditions for models for Aspo Task #5

			CEA/DMT	ITASCA	ANTEA	GOLDER	CRIEPI	BGR	SKB	VTT	ENRESA
Top	Land	water table/inflow near shaft								X	
		no flow/flow after tunnel						X			
		specified flow	X	X	X	X	X		X		X
		fresh					X			X	
	Sea	constant head	X	X	X		X	X			X
		hydrostatic head							X	X	
		head from regional model flow				X					
		sea salinity					X	X	X	X	
Base		no flow	X	X	X	X	X			?	X
		hydrostatic head						X		X	
		head from regional model							X		
		salinity from regional model	X						X		
		brine salinity					X				
		salinity from chemical model									
Sides		hydrostatic head		X			X	X		X	X
		head from regional model	X		X	X			X		
		salinity from regional model	X						X		
		salinity from chemical model								X	
		linear salinity					X				
Tunnel		Specified head	X					X		X	X
		Specified inflow		X	X	X	X		X		

Parameters

- Structural/geometrical information and material properties from Task #3 and Rhén et al (1997)
  - are there significant differences between structural models and properties?
  - various structural adjustments for individual models – how are HCDs connected with measurement points?
  - different approaches to fracture apertures, channelling, background fractures, and rock matrix domain
  - uncertainties in initial and boundary conditions are the predominant issue in Task #5 transport modelling

Parameters



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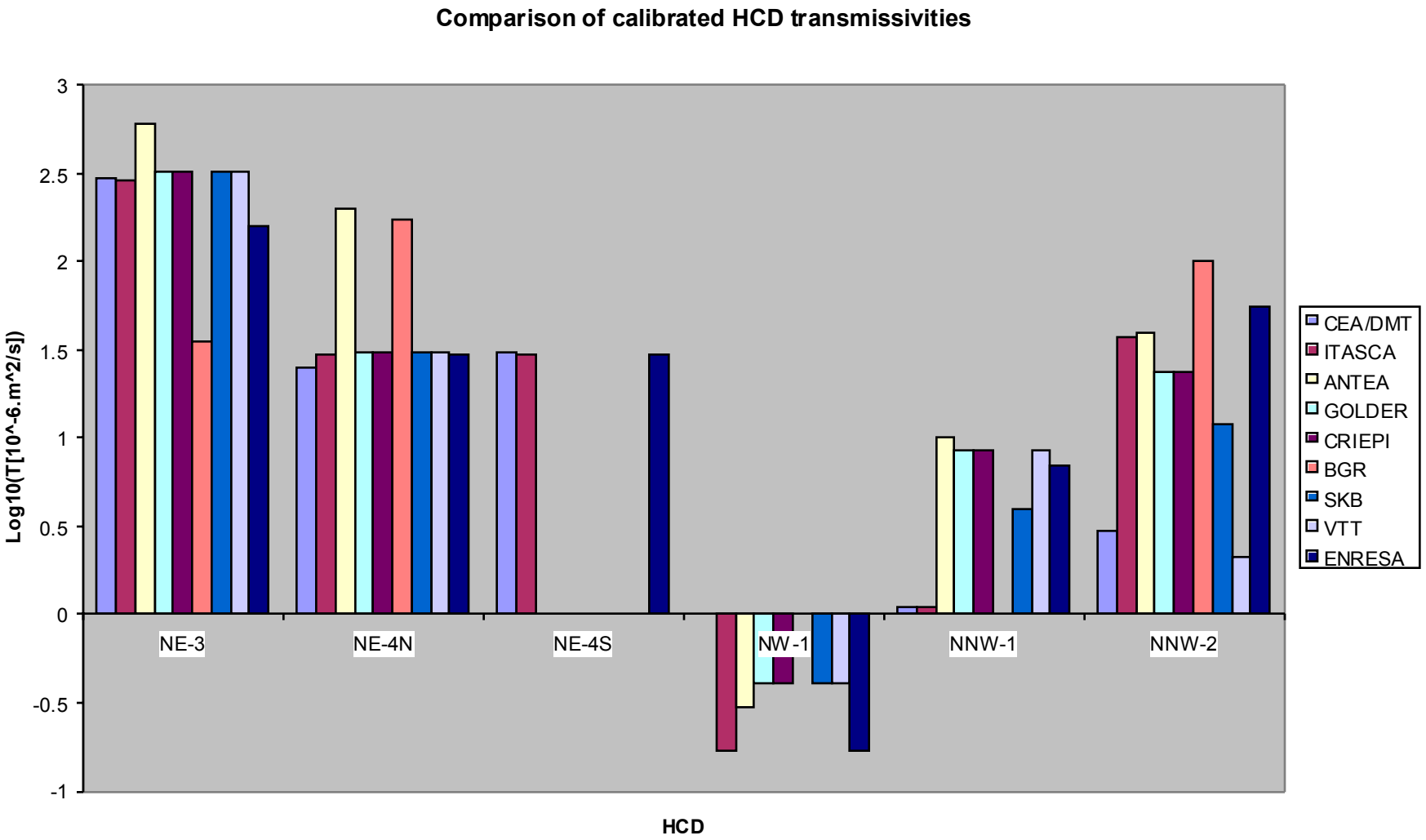

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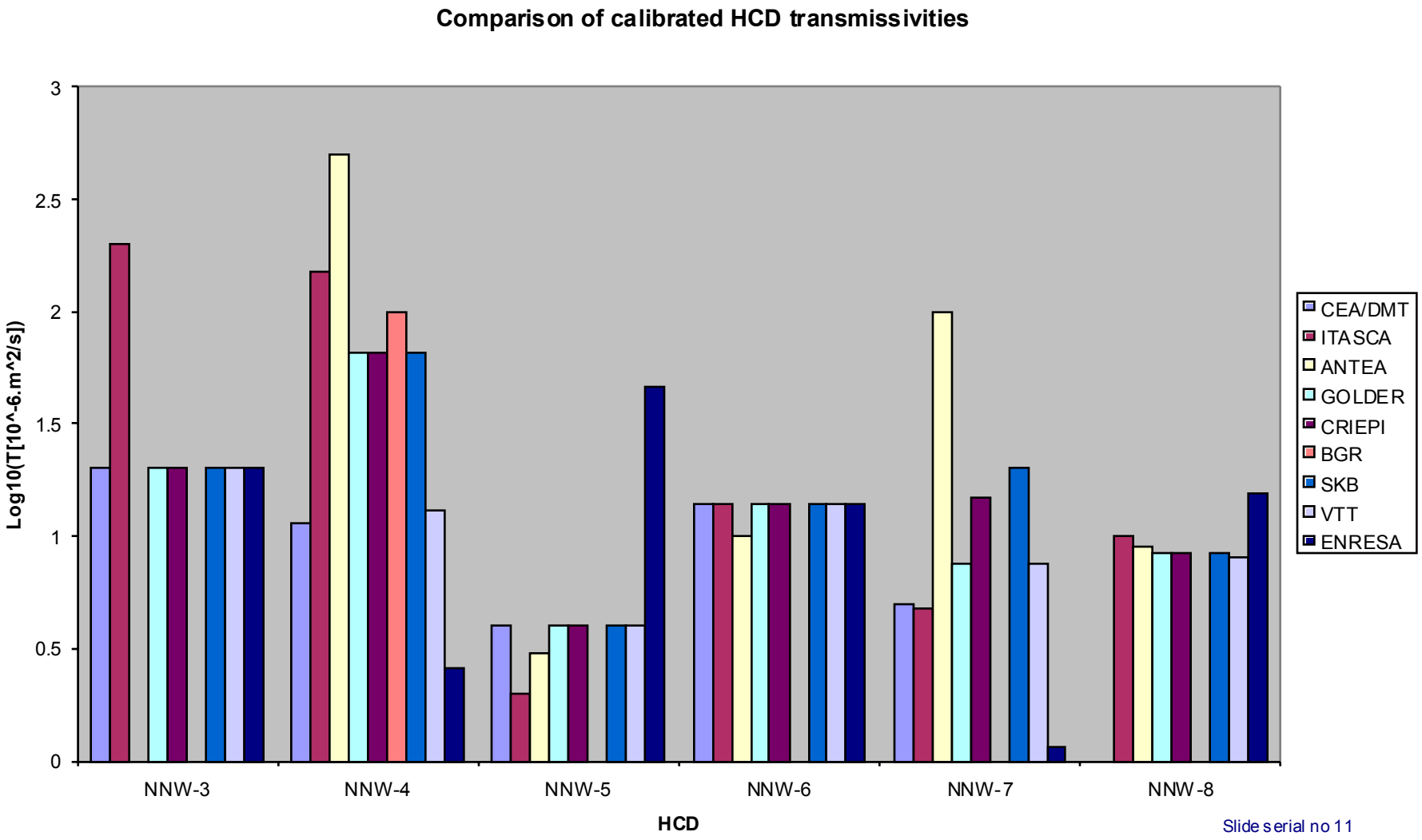
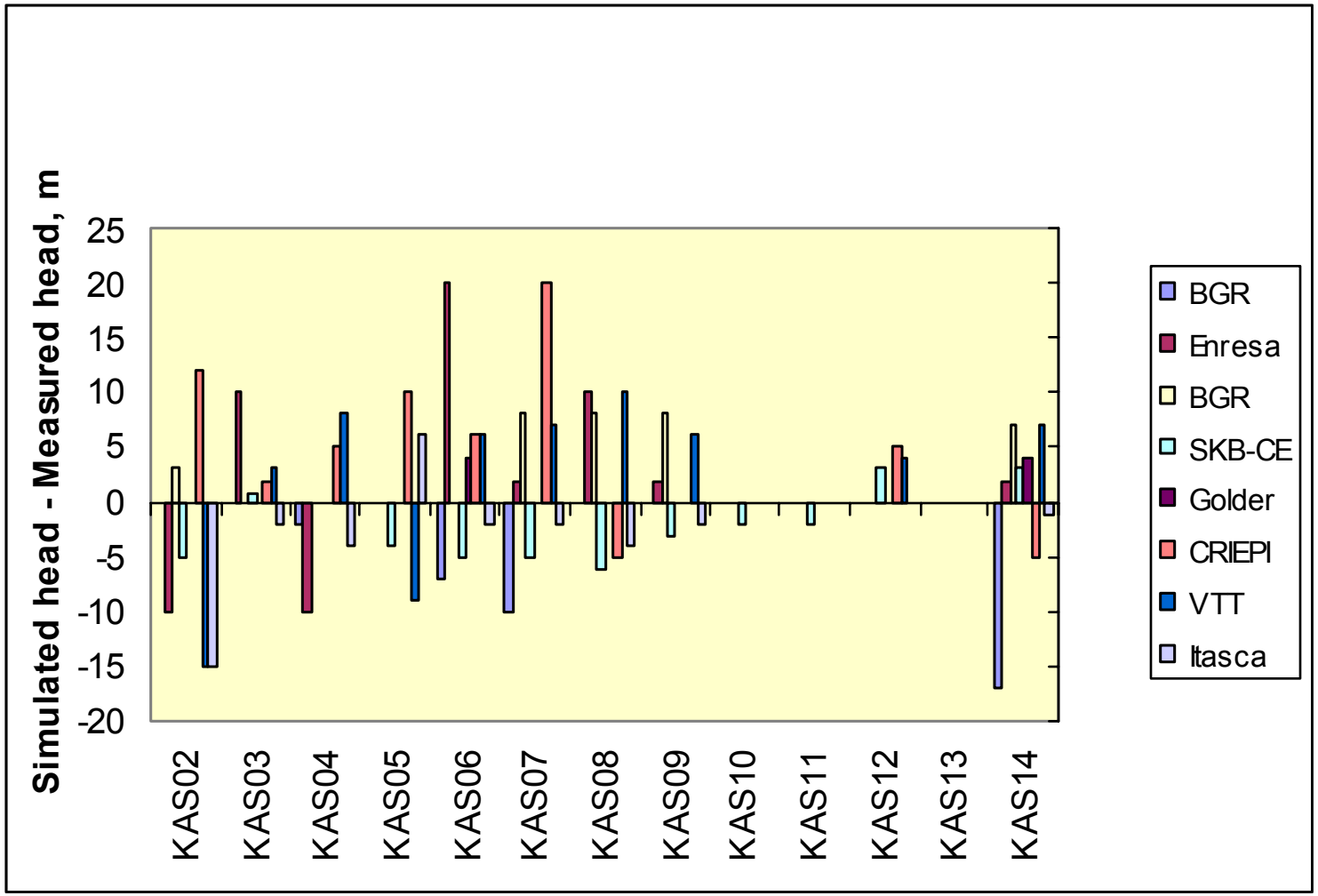


Calibration Approaches

- Calibration approaches vary:
  - initial calibration to heads only or heads + inflows
  - geometrical adjustments and additional features
  - parameter adjustments vary – T, S, n
  - other significant factors – Baltic ‘skin’, recharge
- Different methods for initial and boundary compositions:
  - M3 water types distribution as given
  - regional model (Svensson)
  - various interpolations, kriging and ‘judgement’

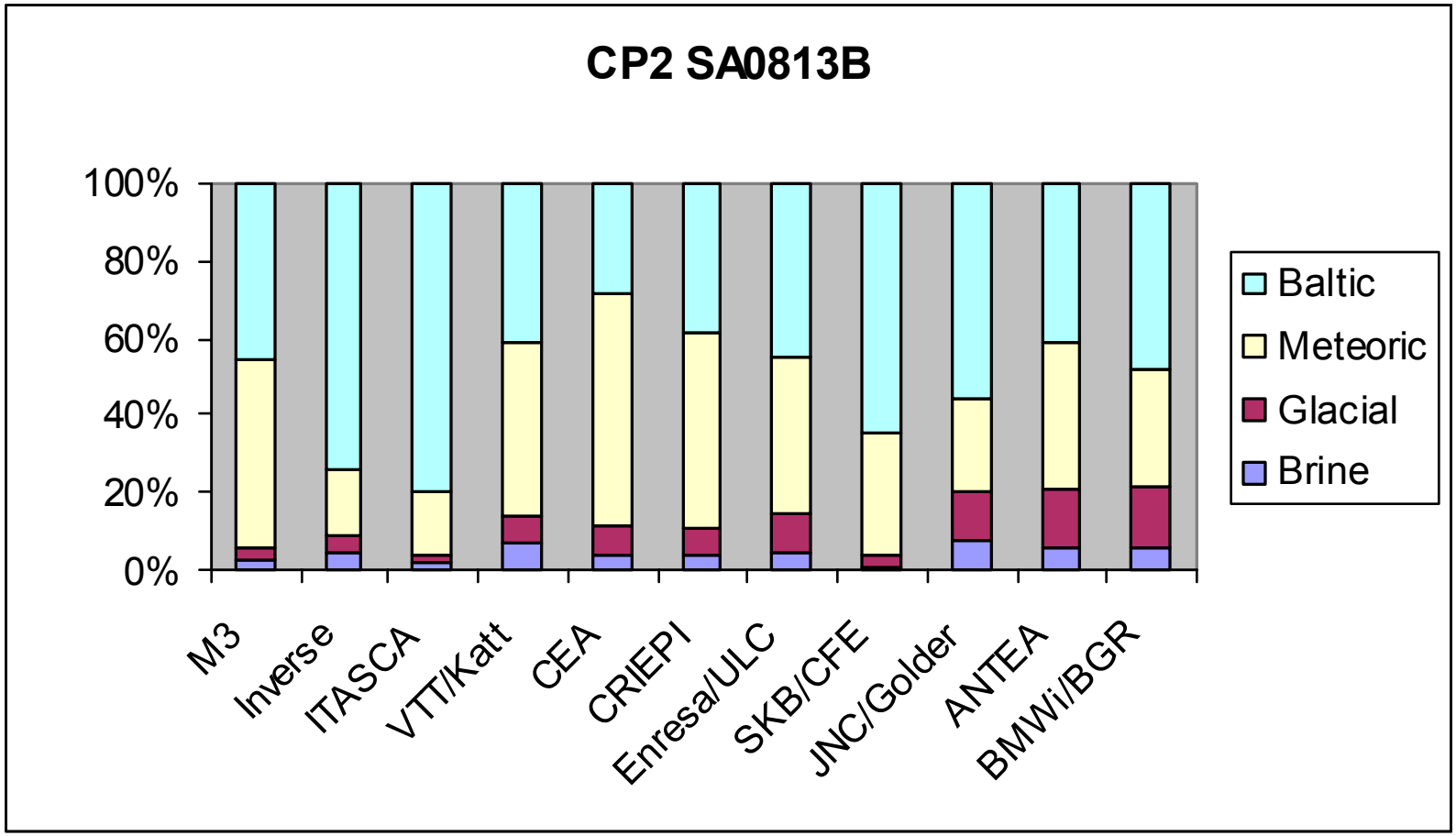
Errors in Calibrated Heads (deep intervals)



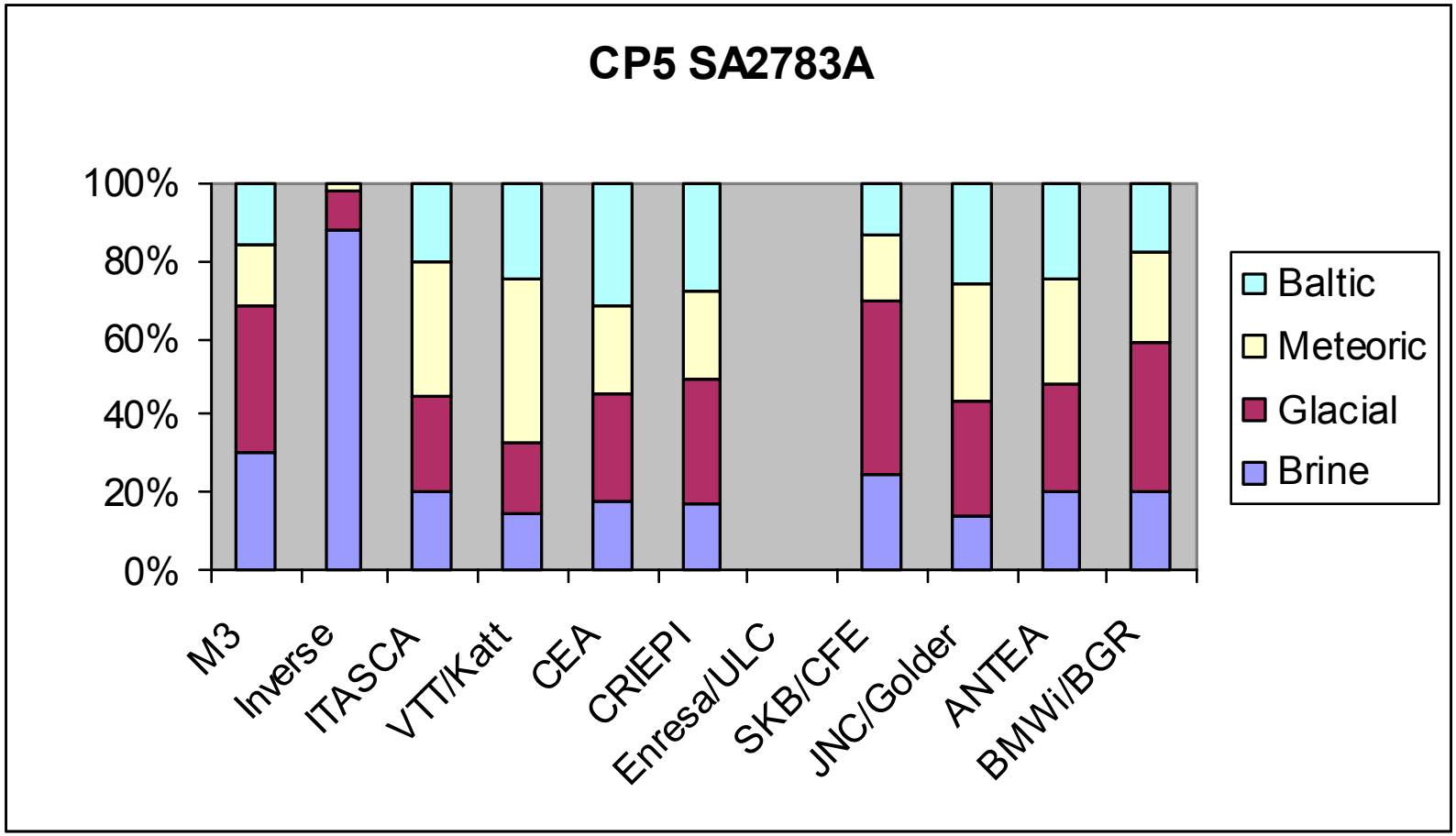
Modelling of Hydrochemical Variations by Mixing

- M3 mixing & mass-balance model
  - identifies 4 water types by PCA analysis of multi-species data; PC plots are resolved into components by a 2-stage mixing model using a 'proxy' mixed 4 component end-member.
- Inverse model
  - identifies 7 water types of which 2 to 5 are components of each measured sample in a 2-stage mixing model, evolving along probable flow paths in Cl-^{18}O space; mass transfers due to mixing are modelled with PHREEQC2.

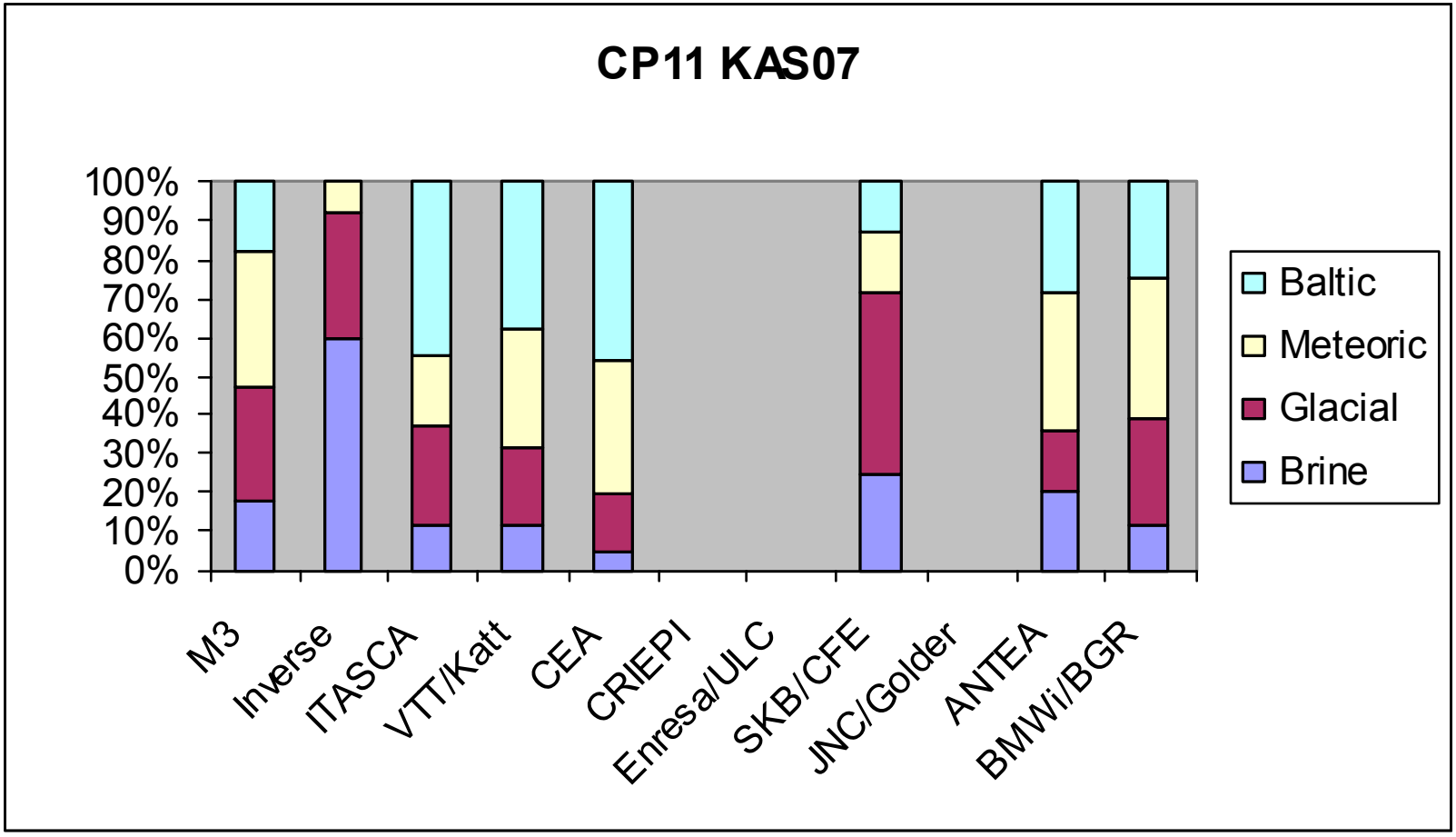
Calculated Mixtures



Calculated Mixtures (continued)



Calculated Mixtures (continued)



Acceptability of Flow-Transport Model

- How credible are the models after calibration and testing?
  - are the parameters and geometry realistic?
  - initial/boundary conditions have significant uncertainties
- Why are there differences between the calibrated models?
  - initial/boundary conditions
  - variations of porosity, connectivity, etc
  - important effect of Baltic sea-bed ‘skin’

Acceptability of Hydrochemical Model

- Reference waters are based on palaeohydrological interpretation of complex evolution
  - this has advantages and disadvantages, and is very site dependent
- Mixing models with >3 end-members are non-unique
  - strongly dependent on Cl and ^{18}O as distinguishing criteria
  - every sample has 4 M3 components – not all are real?
- Two processes may be changing compositions of inflows
  - existing compositions along single flow path or mixing of several flow paths

M3 issues

- Is the M3 approach useful?
- M3 mixing fractions do not obey scalar transport equation
- Would it be better to consider transport of non-reactive species (e.g. Cl, $\delta^{18}O$), or even of the principal components?
- Is mixing dominance real or apparent?
- Is mixing dominant during the perturbation due to tunnel construction?
- Can the M3 approach be used in general?

Calibration issues

- Uncertainties and non-uniqueness
- Relative importance of
  - initial and boundary conditions
  - conceptual model geometry
  - calibration/testing data
- What should be varied and what should be held constant?
  - cross-checks (‘spot checks’) with reality are necessary
  - comparison with long term pump tests?

Confidence-building issues

- Does the available information test the models?
- Why are there differences between the results of the models and the data?
- Are there better experiments to test the models?
- Upscaling of the models and applicability to Performance Assessment – what has been learnt?

Other Issues

- Flow, solute tracing and water mass mixing: are they compatible in an excavation experiment?
- Presentation of input and output data
- Geochemical reactions: is there confirmatory evidence?
- Propagation of uncertainties in models

Have the objectives been achieved?

- To what extent are flow and mixing-reaction models consistent, and is there a possibility of using this further to improve confidence in PA models of a repository system?
- What lessons have been learned about integrating hydrogeological and hydrochemical data in assessment of sites under both disturbed (i.e. excavated) and undisturbed (i.e. post-closure) conditions?

Have the objectives been achieved? (continued)

- What would be the recommended methodology for integrating hydrogeological and hydrochemical data?
- In general, how has Task 5 increased knowledge and understanding of groundwater in fractured rock?

Recommendations

- Importance of ‘baseline’ data for initial/boundary conditions
- Duration of monitoring period and acquisition of data to test models)
- Selection of hydrochemical data and minimisation of uncertainties
- Modelling approach
- Calibration procedure and quality of model testing
- Benefits of multiple teams

Supplementary Task 5 modeling

Shuttle (Golder) et al

Supplementary Task 5 Modeling

Äspö Modeling Task 5 Meeting
16 November, 2000

Dawn Shuttle/Golder
Bill Dershowitz/Golder
Masahiro Uchida/JNC-Tokai
Richard Metcalfe/JNC-Tono
Mark Cave/BGS

JNC サイクル機構

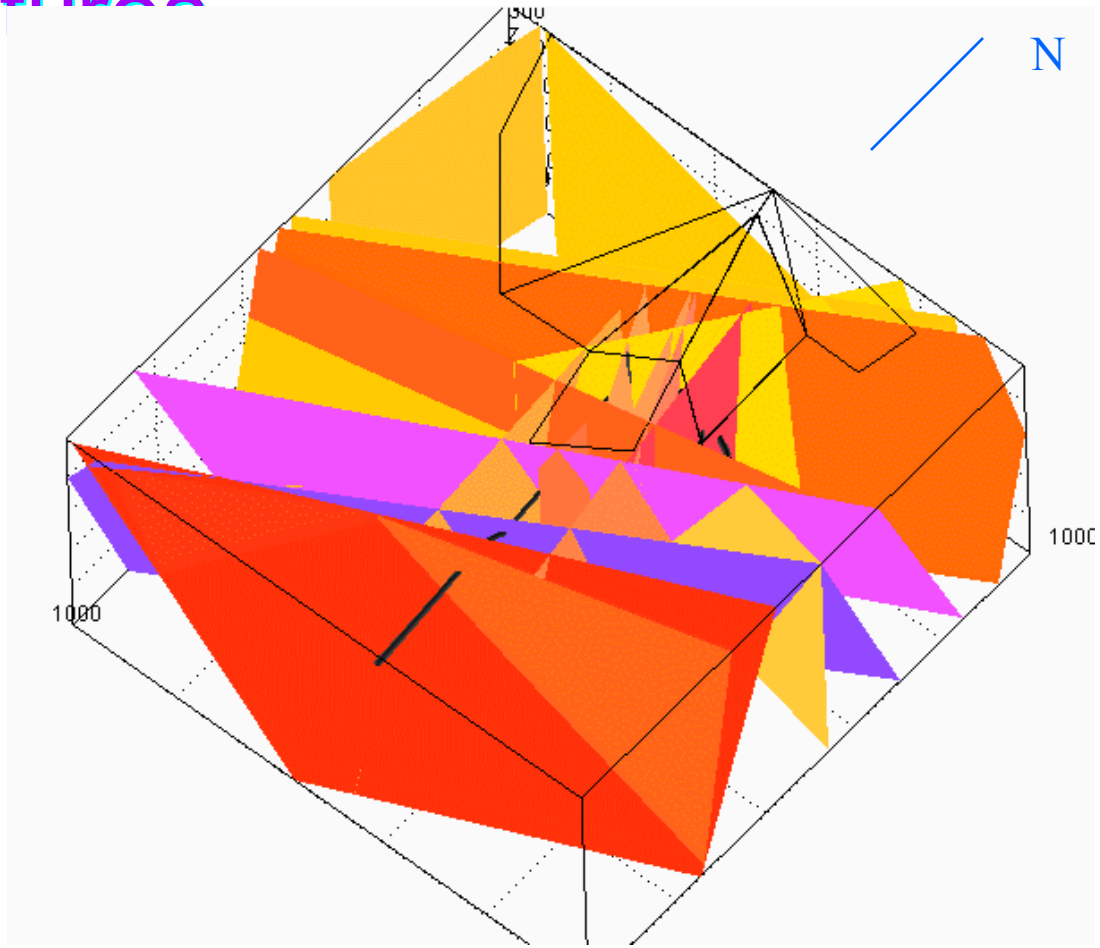
JNC/Golder Task 5 Goals and Approach

- Demonstrate the Value of Geochemical Data for Construction and Validation of Hydrogeological and Pathway Models
- Stage 1: Calibrate and Predict Based on Hydrological Data Only (Results Presented 4/99)
- Stage 1.5: Calibrate and Predict Based on Hydrological Data Only (10/99)
- Stage 2: Update based on Geochemical Data, Repeat Predictions (10/99)
- Stage 3: Complementary Analysis to Address Uncertainty Issues (11/00)

JNC/Golder Task 5 Reporting

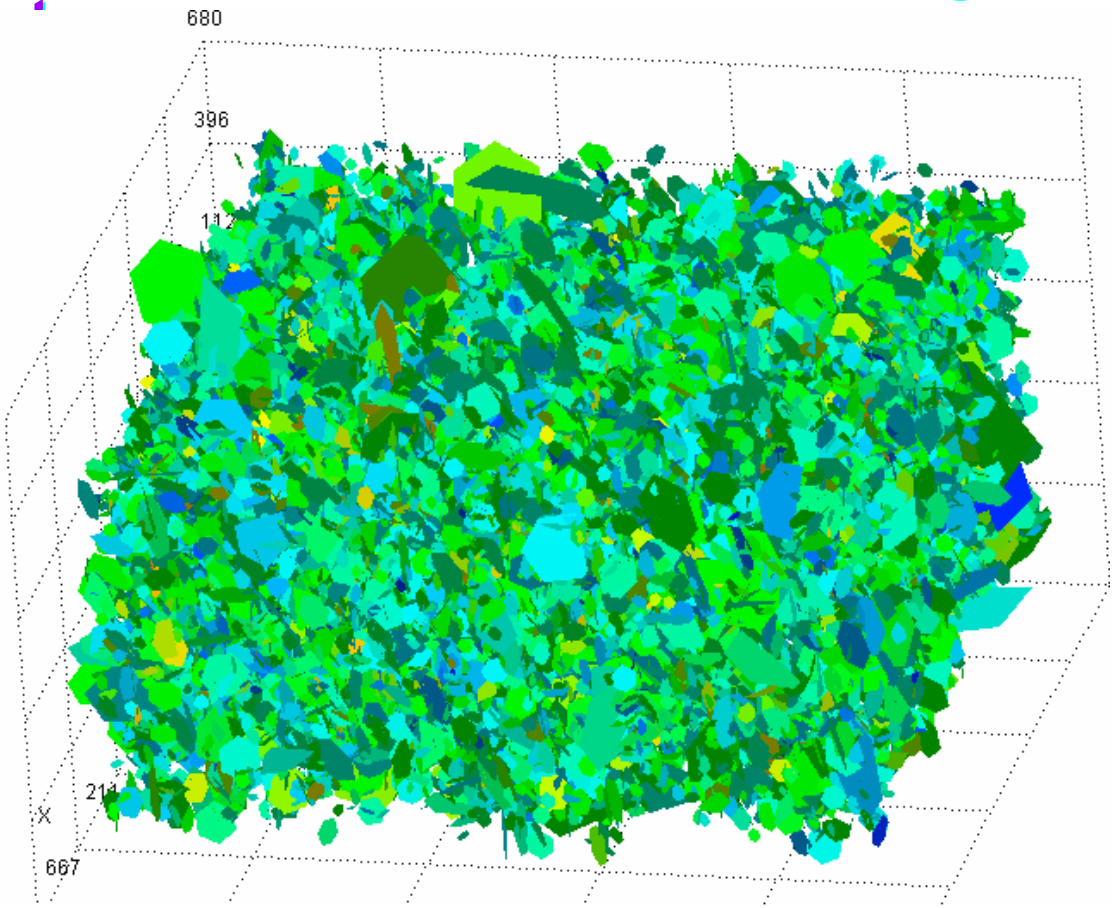
- Approaches, Algorithms, and Demonstration
  Report Dated 12/98
- Hydrological and Geochemical Calibrations and Predictions
  Report Dated 12/99
- Complementary Analysis to Address Uncertainty Issues
  Report Dates 12/00

Task 5 DFN Model - Large Scale Features



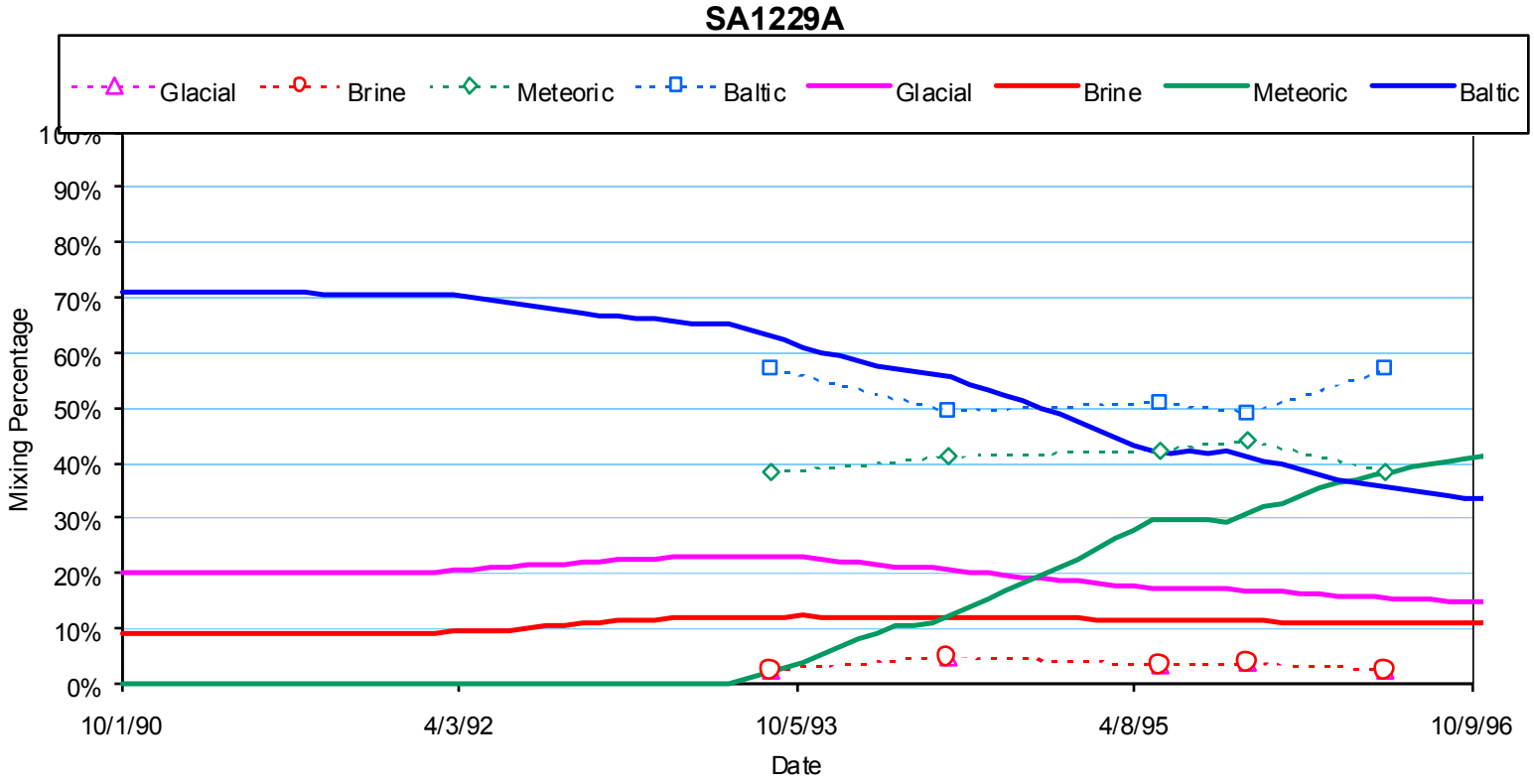
JNC サイクル機構

Task 5 DFN Model - Background Fr



JNC サイクル機構

Typical Result from 1999 Task 5 Model



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Issues to be addressed

- Uncertainty introduced to the analysis by the use of the four M3 geochemical endmembers
  ---> Multivariate Analysis for endmembers with lower residual error
- Pathway analysis limitations based on graph theory algorithm
  ---> New particle backtracking algorithm to improve pathway identification
- Spatial interpolation of initial conditions
  ---> Interpolation weighted to reflect fracture zone geochemistry patterns, and to distinguish waters under Aspo island from those beneath the Baltic

Geochemical Endmember Analysis M3

	Na	K	Ca	Mg	HCO3	Cl	SO4	O18	D	Tr
Brine ref. w.	8500	45.5	19300	2.12	14.1	47200	906	-8.9	-44.9	4.2
Baltic Sea ref. w.	1960	95	93.7	234	90	3760	325	-5.9	-53.3	42
Glacial ref. w.	0.17	0.4	0.18	0.1	0.12	0.5	0.5	-21	-158	0
Meteoric ref. w.	0.4	0.29	0.24	0.1	12.2	0.23	1.4	-10.5	-80	100

Endmember Analysis
JNC/BGS Multicomponent Analysis

Model 2 Component	Na	K	Ca	Mg	HCO3	Cl	SO4	O18	D	Tr
1	8508.6	5.1	17235.0	0.0	47.1	44001.5	800.3	-11.8	-75.7	14.6
2	2066.3	0.0	1379.1	169.1	225.4	6163.5	0.0	-8.8	-68.5	0.0
3	456.9	5.5	258.4	16.7	0.0	1207.9	79.8	-12.4	-94.2	0.0
4	0.0	1256.2	0.0	2020.1	505.6	0.0	0.0	0.0	0.0	492.0
5	0.0	0.0	0.0	0.0	22039.5	0.0	0.0	0.0	0.0	0.0
6	0.0	0.0	0.0	0.0	298.8	0.0	0.0	0.0	0.0	391.5
7	2021.3	17.8	205.4	8.0	0.0	3230.3	1284.4	-14.3	-107.9	0.0

Mark Cave/BGS with Richard Metcalf/JNC

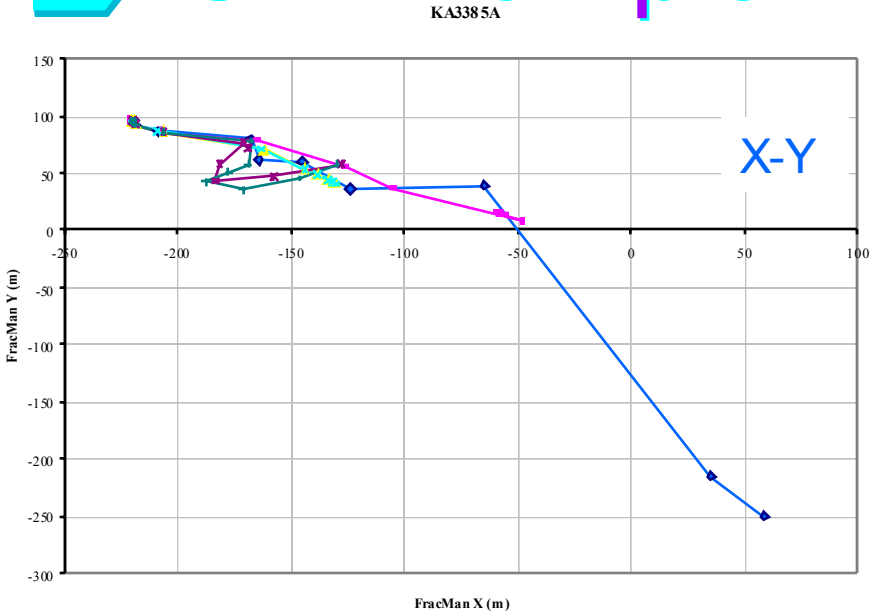
Pathway Analysis

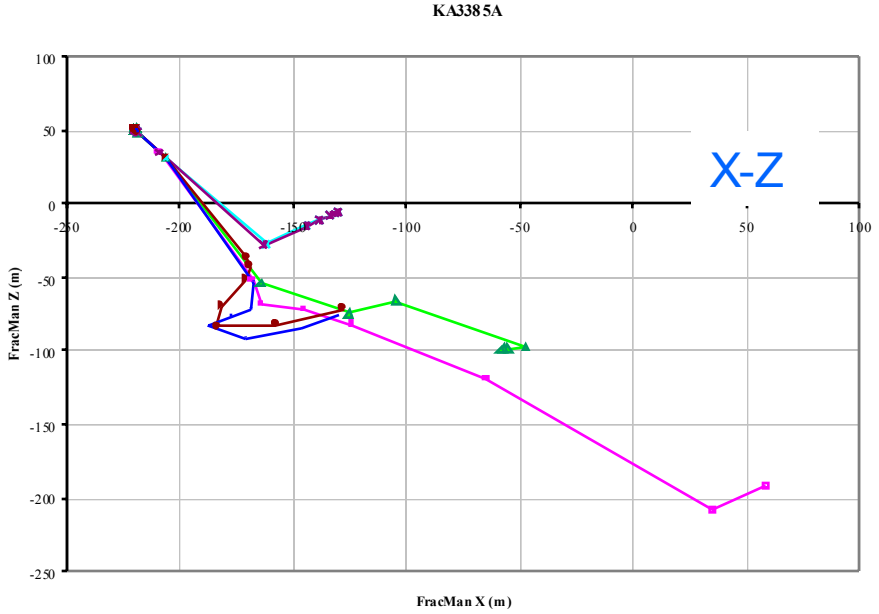
- Graphical pathway analysis (JNC, 1999) identified pathways for the final, "steady state" head field, then moved mass down those pathways based on transient heads for 76 30-day time steps.
- Particle back-tracking algorithm follows pathways through the transient head field as it develops through the 76 time steps
- Particle back-tracking algorithm that uses the "upgradient" network from the sampling borehole interval to the outer boundaries of the model

Transient Particle Backtracking Analysis

- Algorithm stochastically distributes particles at pipe intersections in proportion to the pipe flow rates.
- Advantage of this algorithm is that the upstream network finds all possible pipes. Therefore provided enough particles are used, results include all potential pathways in the finite element model.

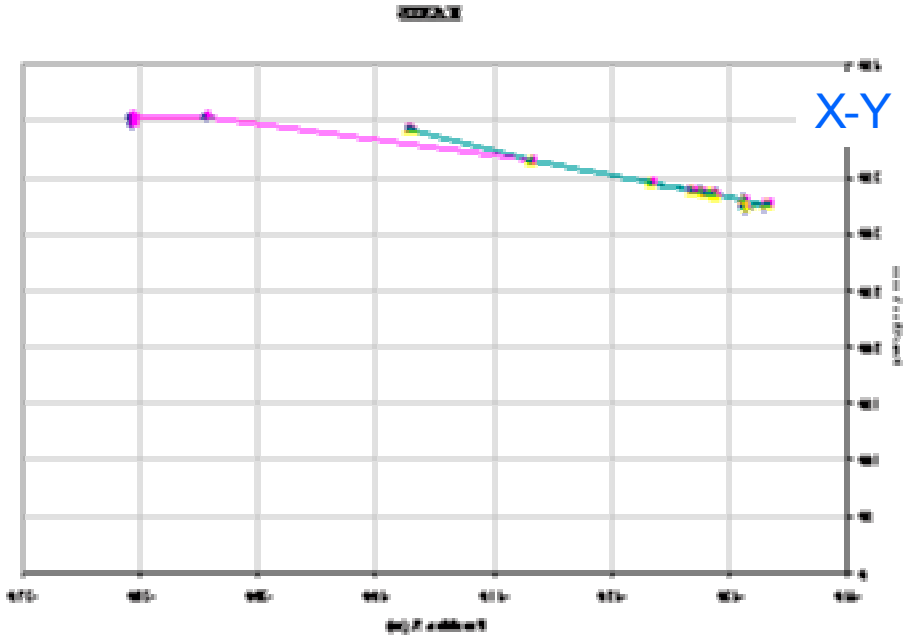
Six Example Pathways for KA3385

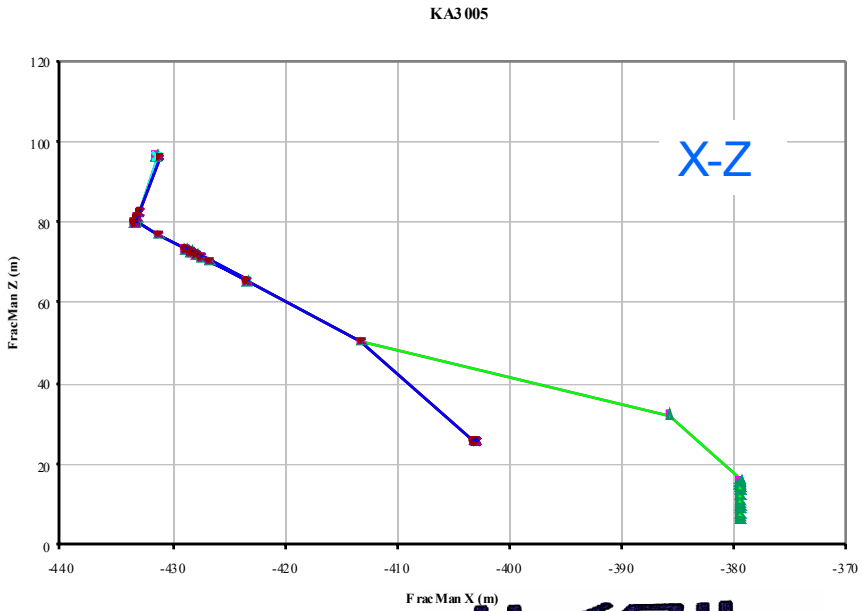




JNC サイクル機構

Six Example Pathways for KA3005





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Interpolation of Initial Geochemical Conditions

- Previous analysis used a form of kriging to distribute geochemical endmembers according to a spatial grid from the limited borehole sample locations
- Updated analysis assumes that the original chemistry in the background fractures is similar to the chemistry in adjacent major fracture zones to achieve what we hope is a more realistic initial condition

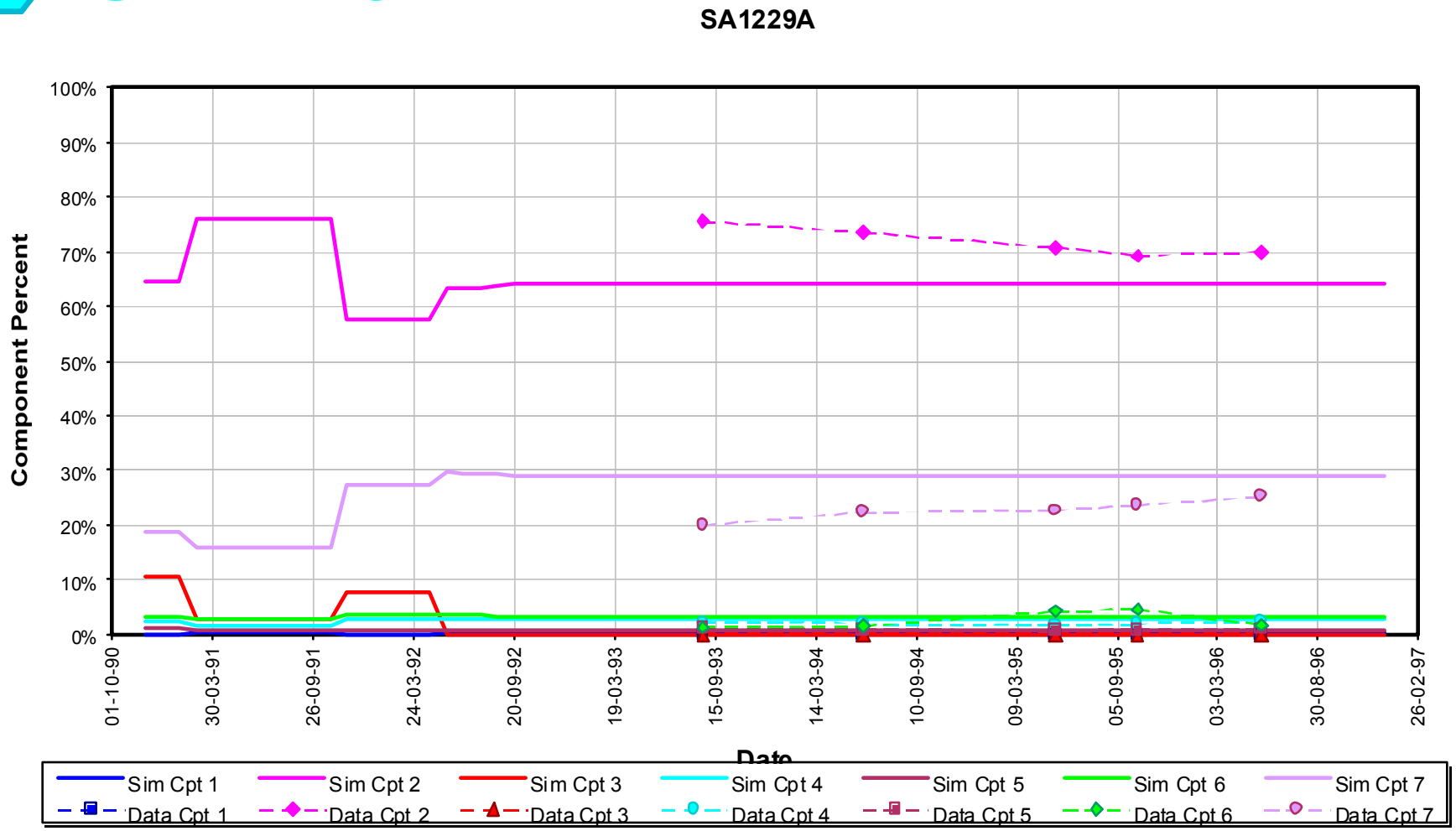
Geochemistry Initial Condition Interpolation Algorithm

- Step 1: Project measured chemistry to adjacent major fracture zones.
- Step 2: Obtain location of particle using the PAWorks particle backtracking algorithm
- Step 3: If particle is not within a main fracture zone, project particle to the nearest zone
- Step 4: Interpolate chemistry from the chemistry on these fracture zones

Geochemical Initial Conditions
Interpolation Algorithm Assumptions

- For particles under Aspo Island, the interpolation was carried out using measured chemistry from under Aspo Island.
- For particles under the Baltic, the interpolation was carried out using measured chemistry from under the Baltic.
- This interpolation approach is limited by the number of available data points.

SA1229A



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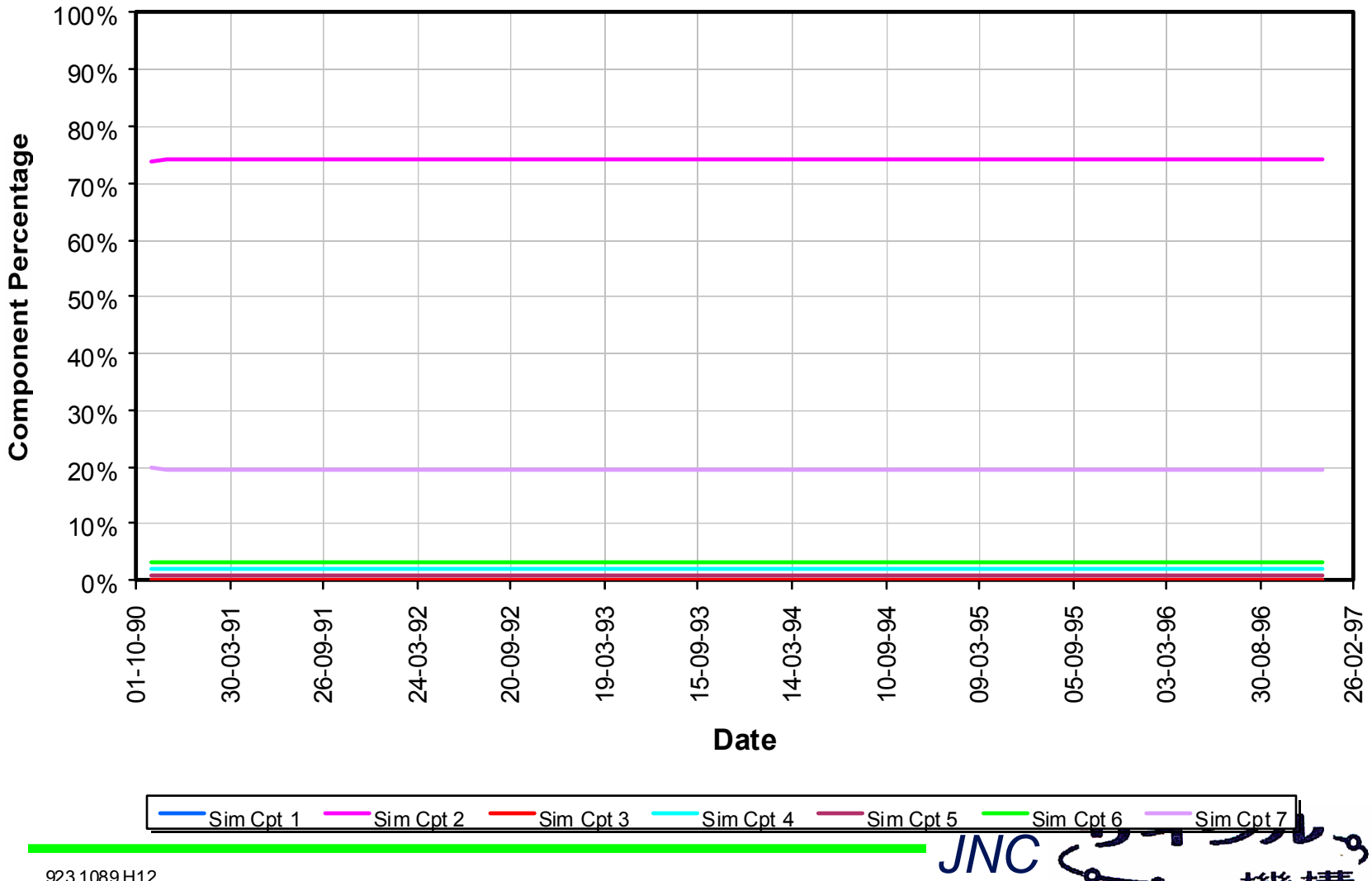

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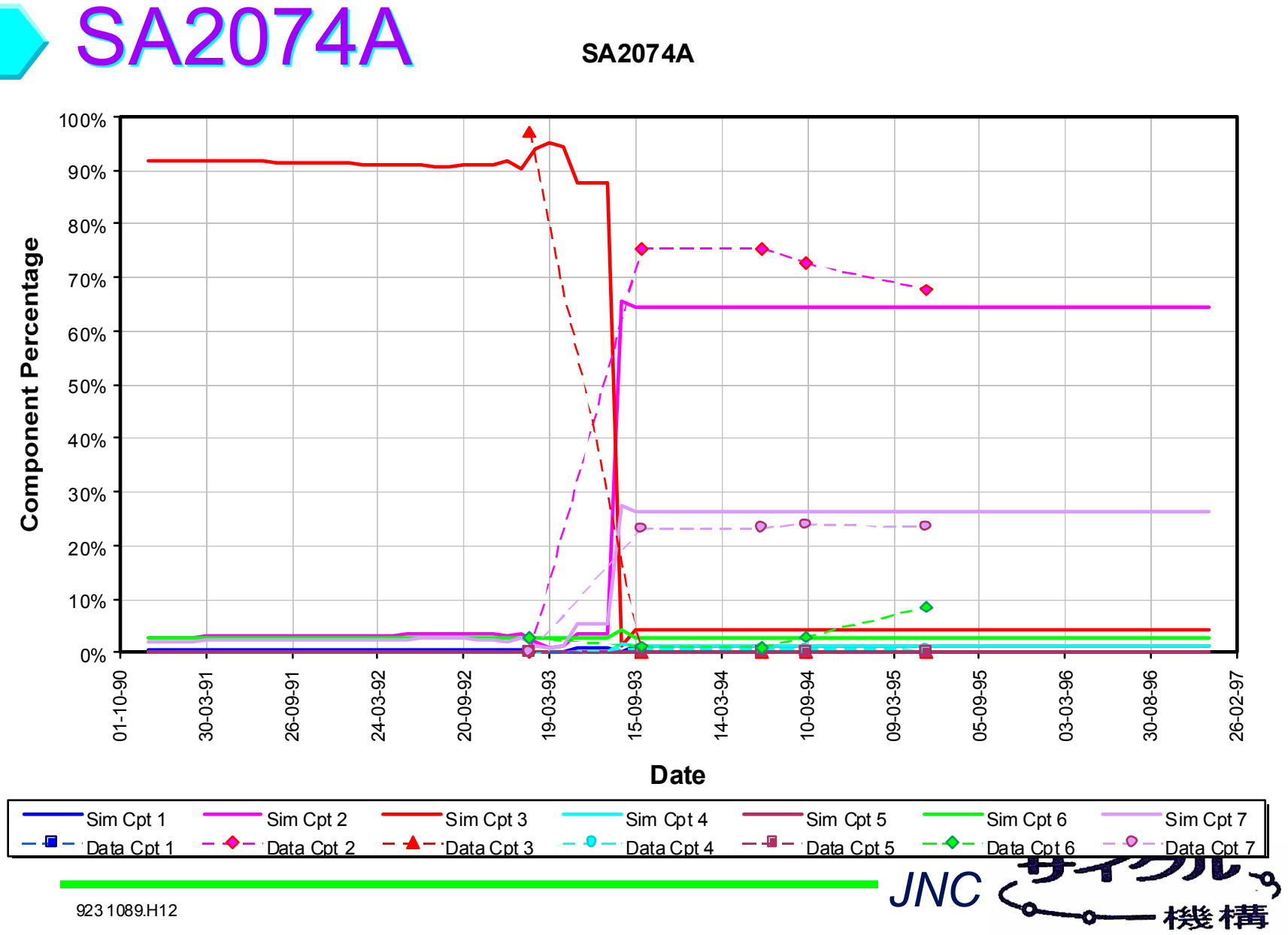

JNC サイクル機構

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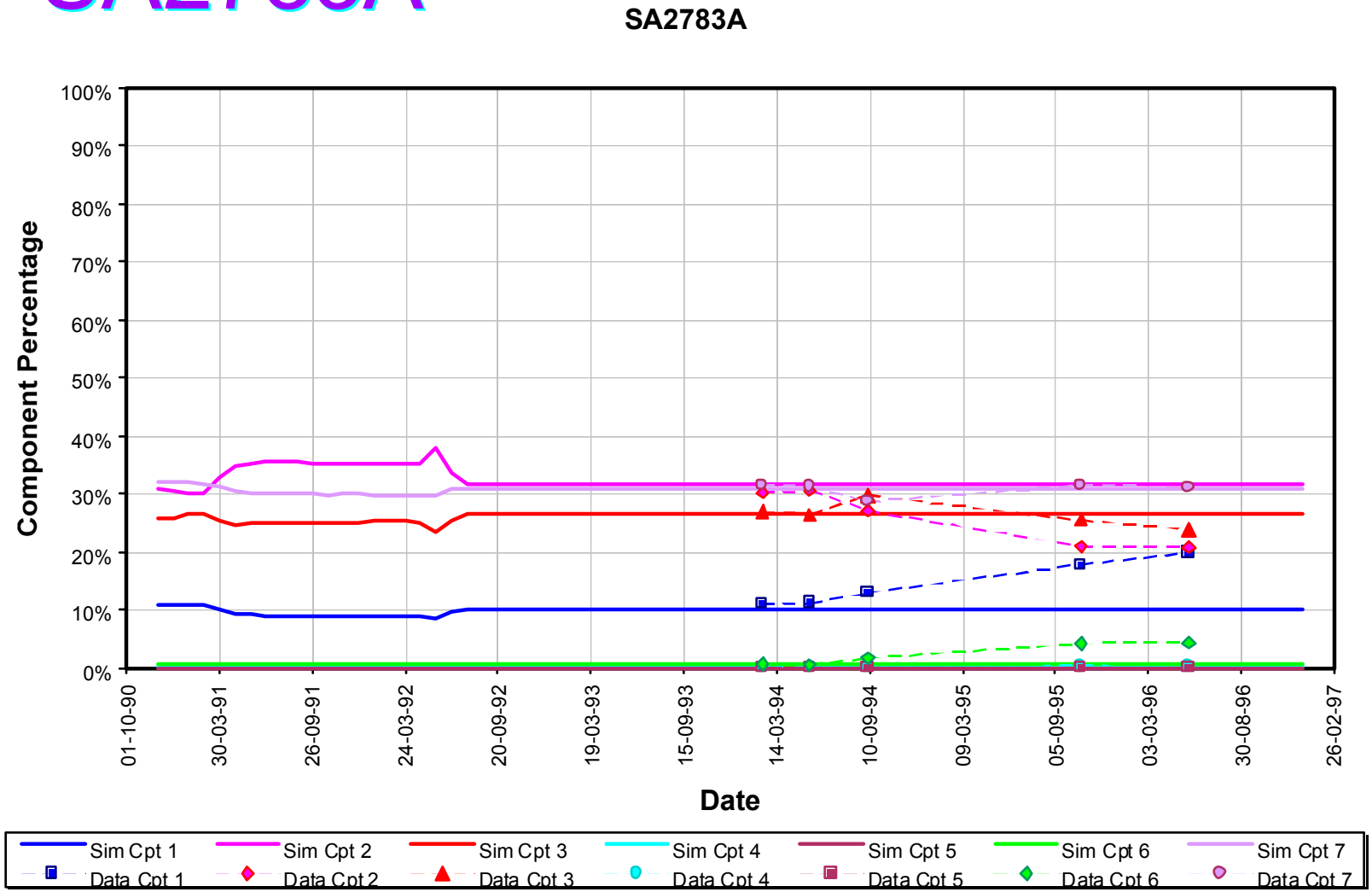

JNC サイクル機構

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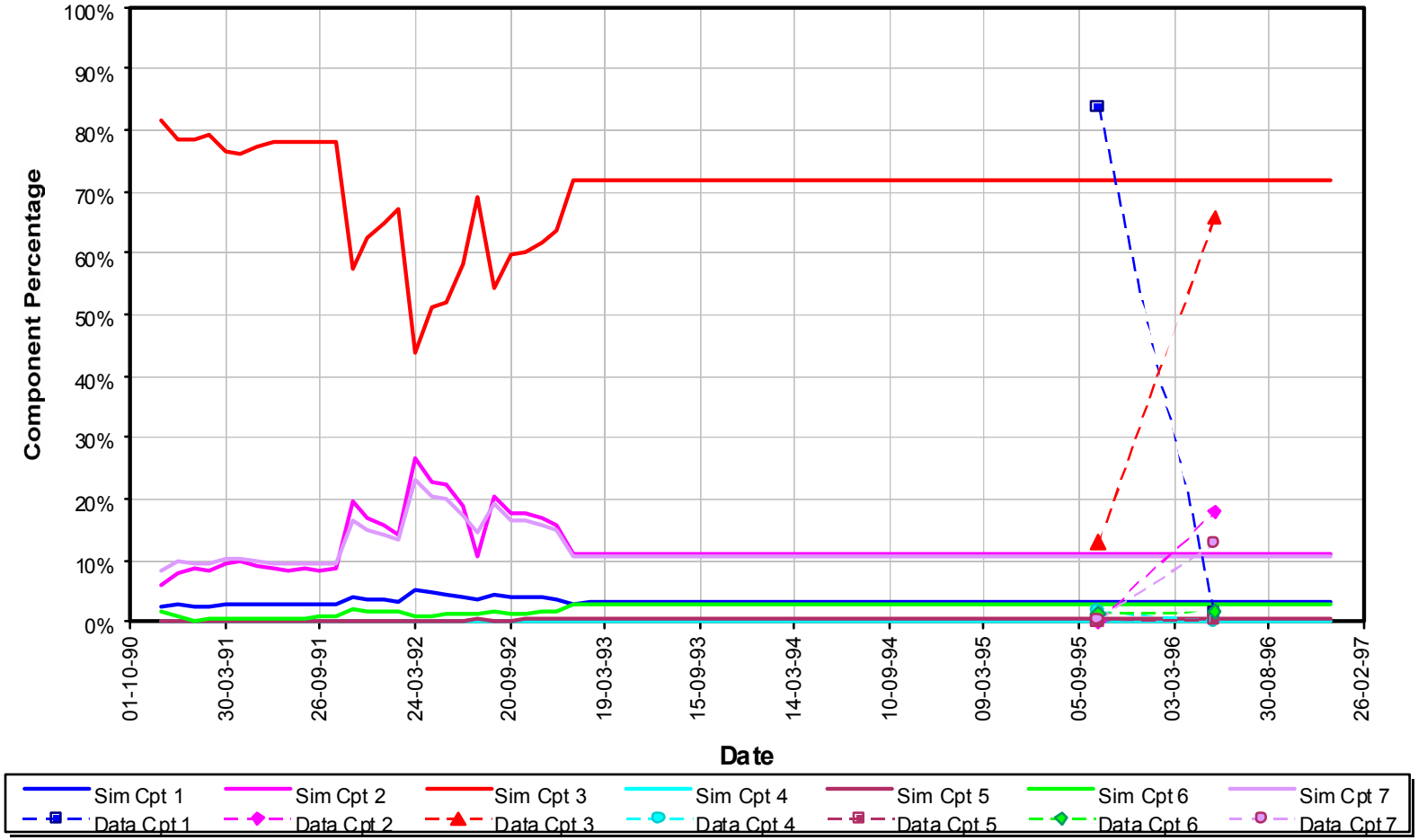

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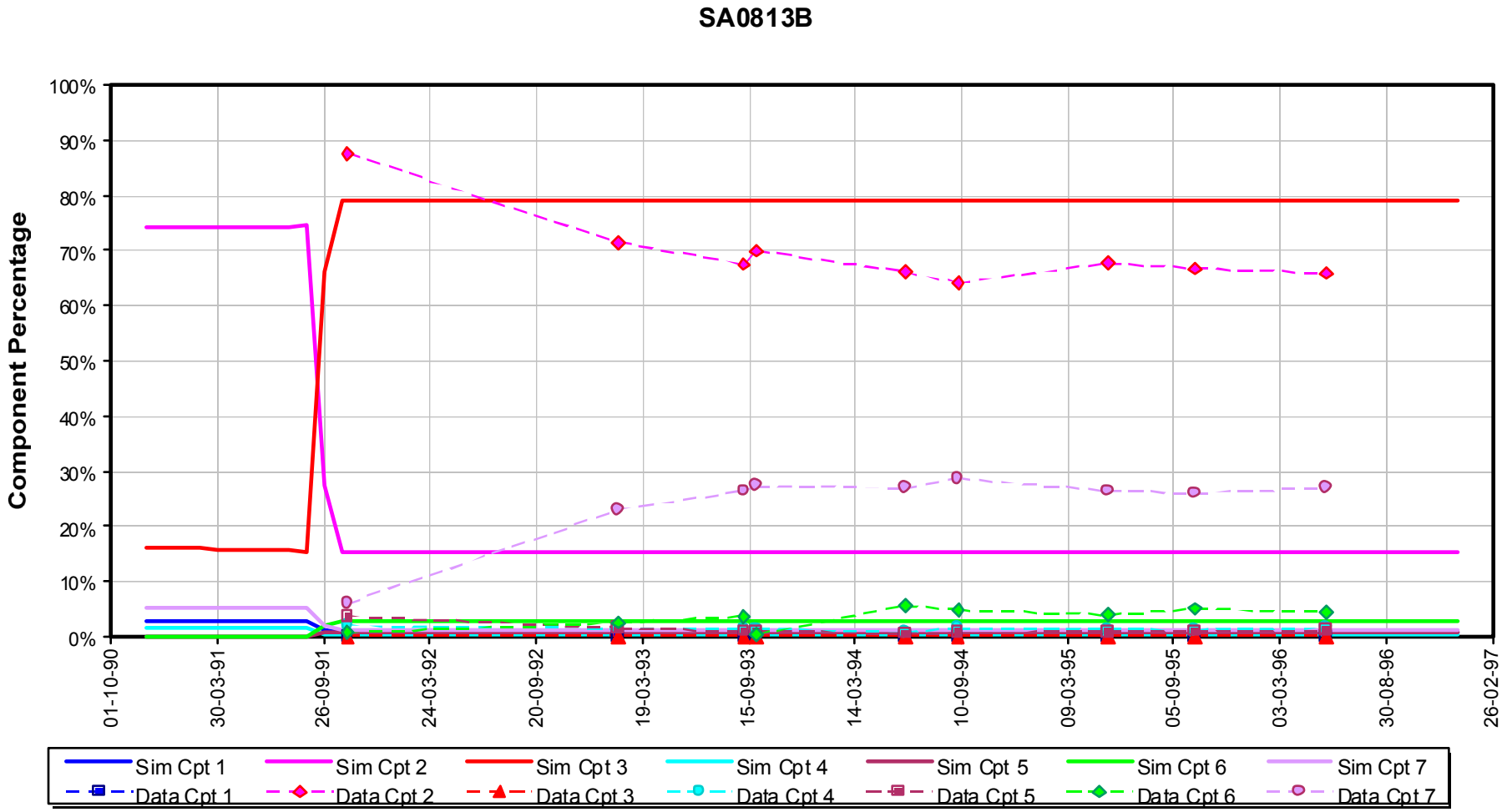

JNC サイクル機構

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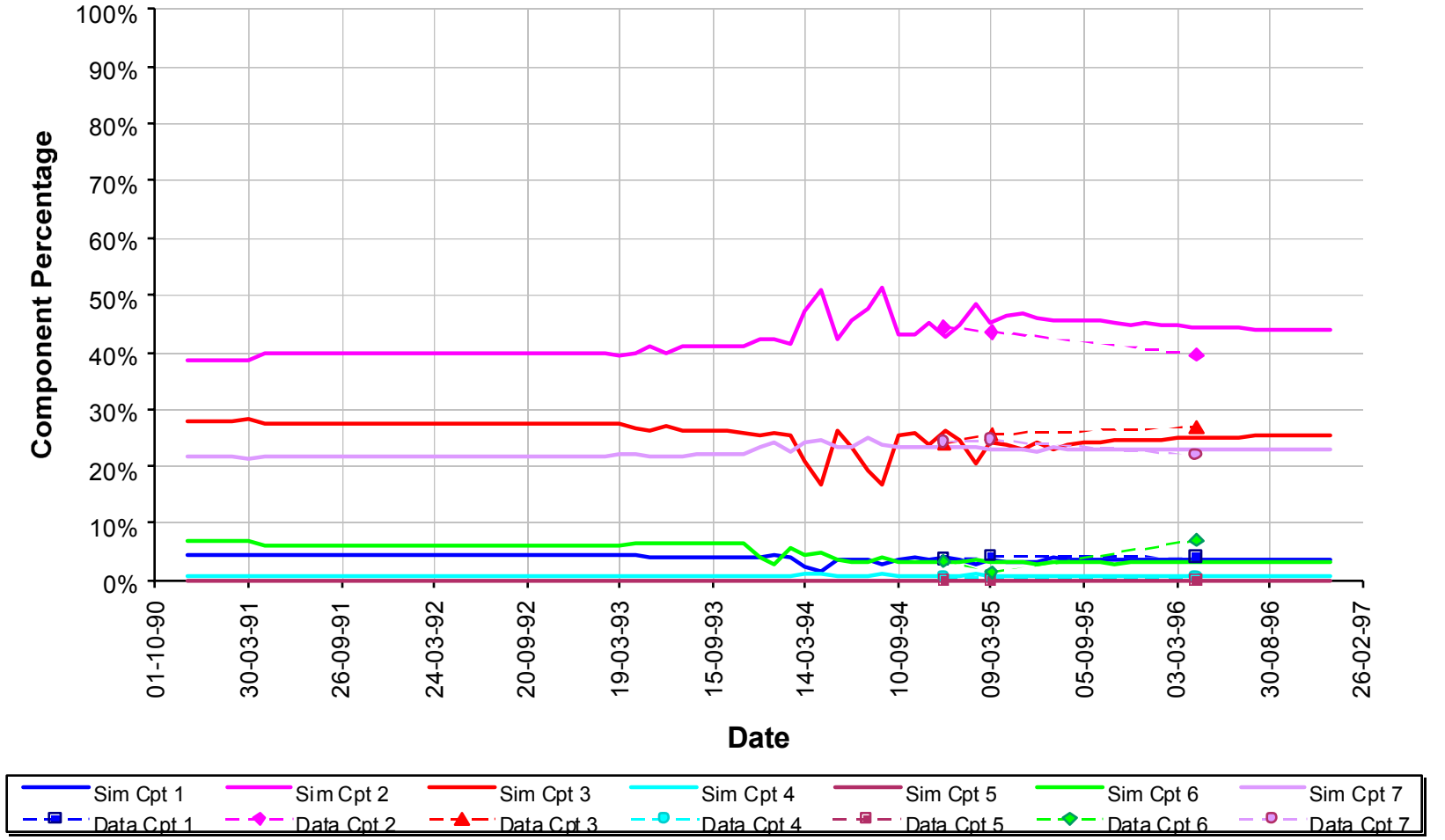

JNC サイクル機構

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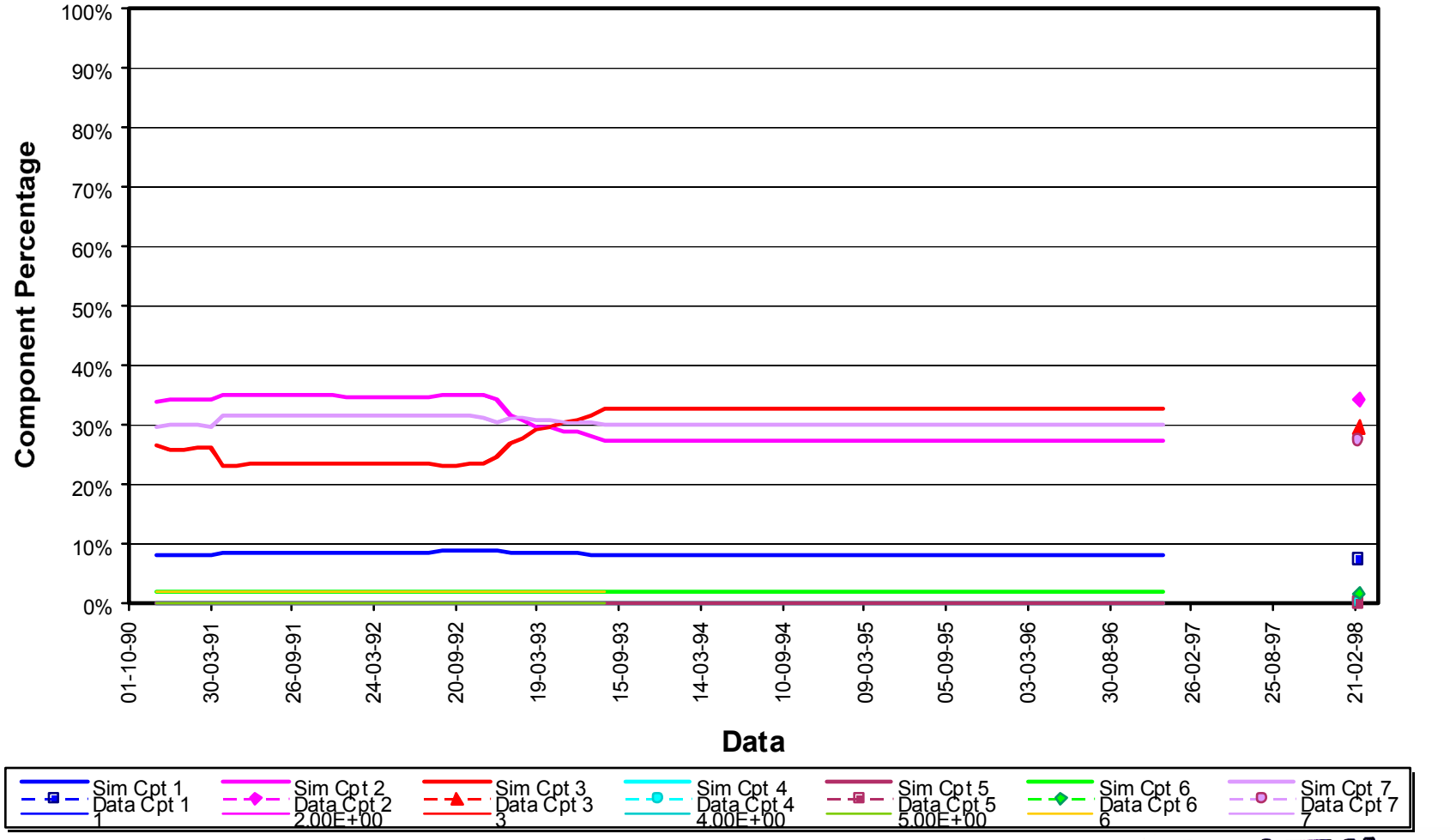
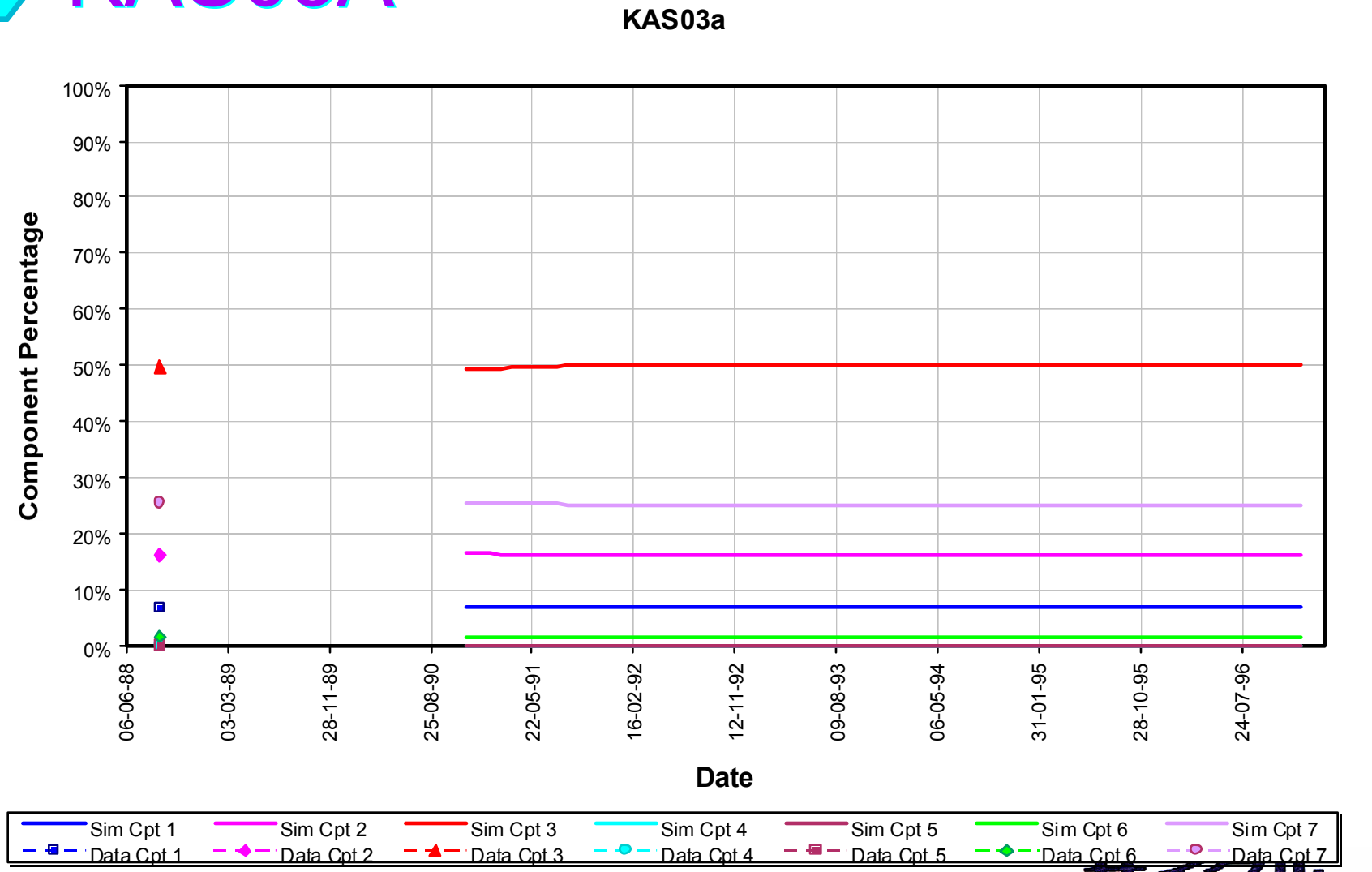


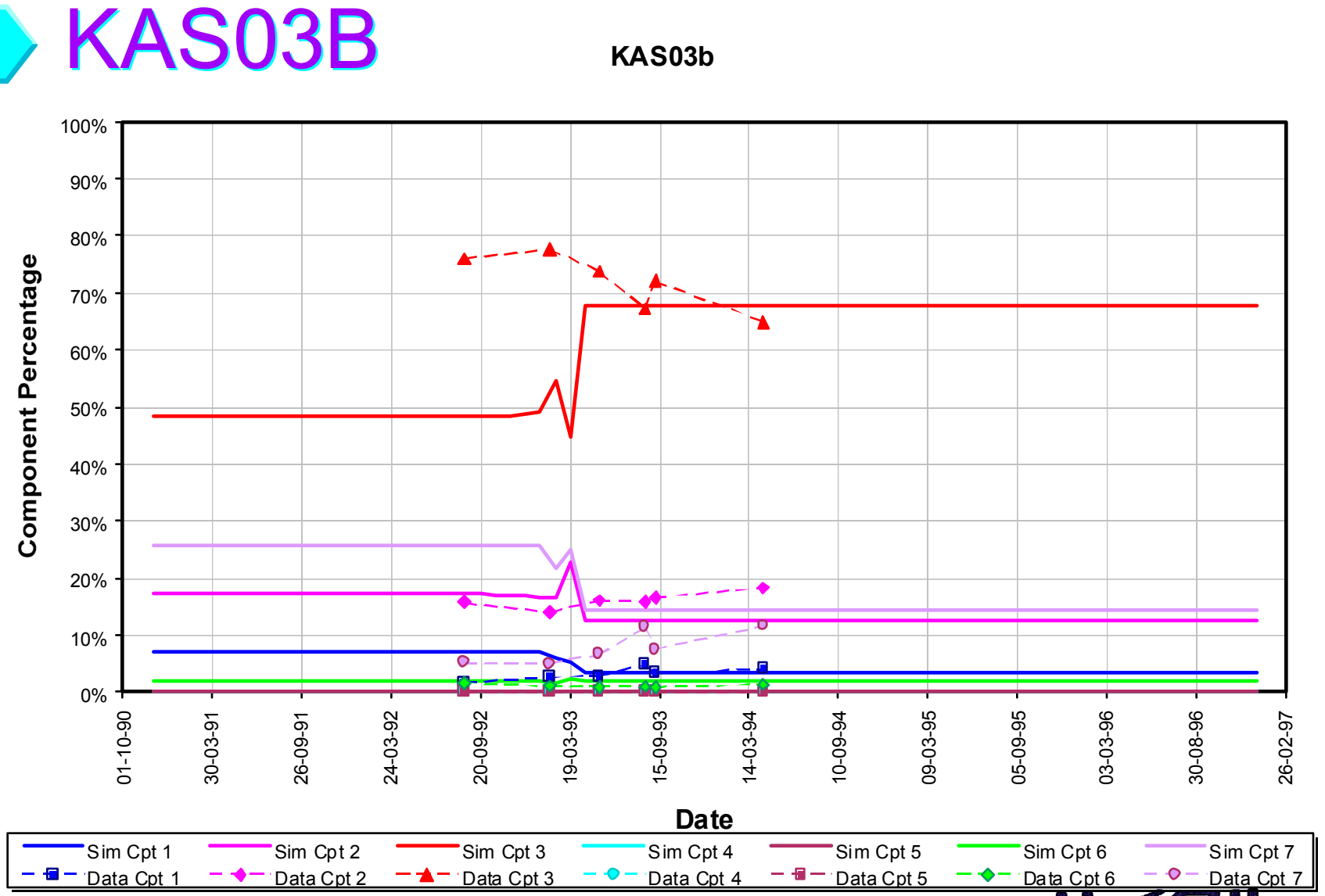
JNC サイクル機構

KAS03A



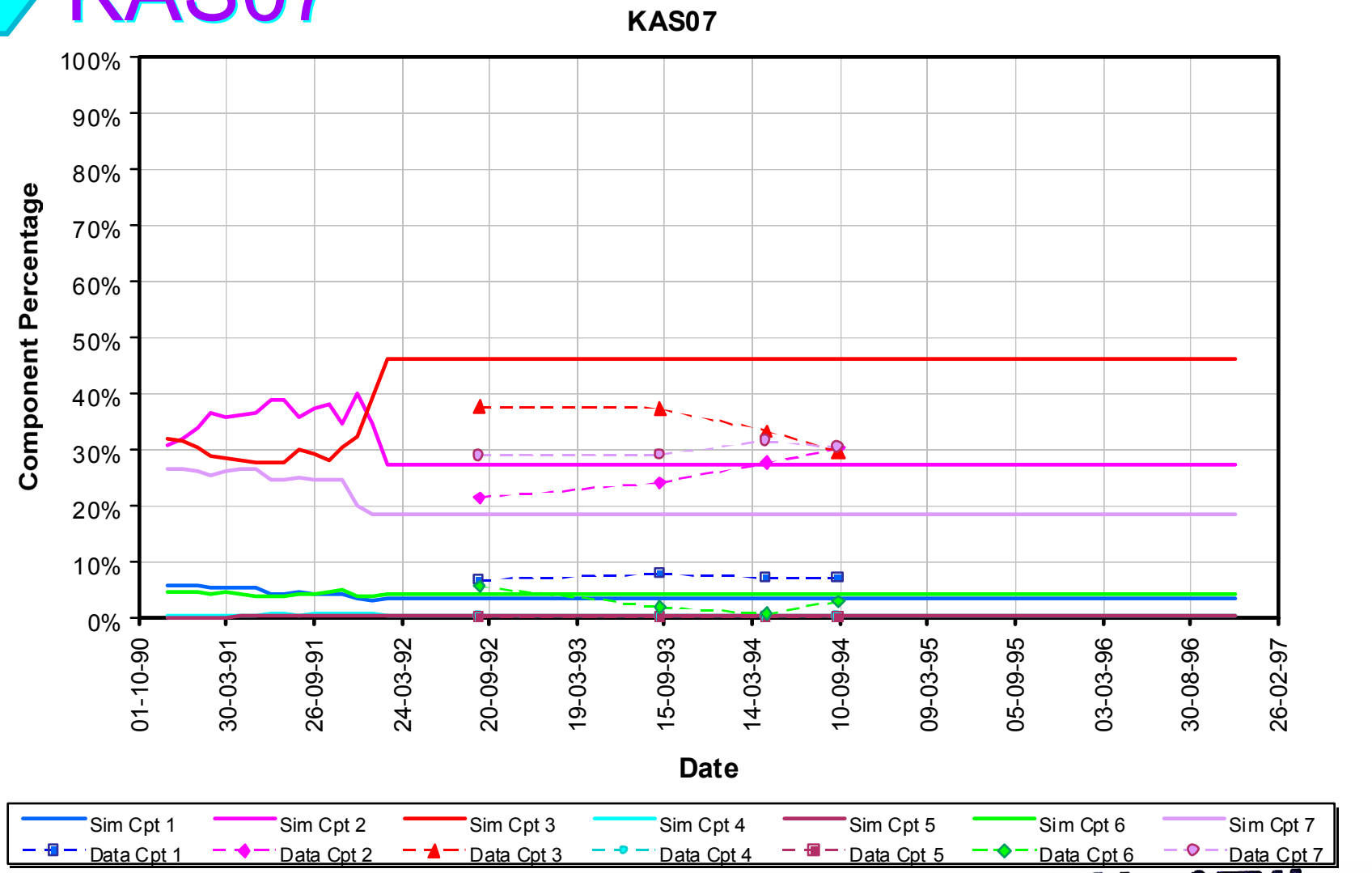
JNC サイクル機構

KAS03B



JNC サイクル機構

KAS07



JNC サイクル機構

Conclusions

- Signifiant Improvements in Breakthrough Calibration
- Interpolation for Spatial Distribution of Endmembers is the Key to Task 5
- Seven "Principal Component" Endmembers better match actual Chemistry, but lack meaning
- Improved Pathways Identification Analysis: Potentially Useful for PA

Appendix G

Task 6 proposal

J-O Selroos (SKB)

Task 6 proposal: Performance Assessment Modelling Using Site Characterisation Data (PASC)

Benabderrahmane/Dershowitz/Selroos/Uchida/Winberg

Background

- Task 6 will focus on the 50 to 100m scale which is critical to PA according to many repository programs.
- PA models are simpler and physically less realistic than SC models.
- Usefulness of in situ tracer experiments for PA (issue listed at 1st GEOTRAP workshop 1996)?
- Bridge the gap between PA and SC models by applying both approaches for the same tracer experiment, and also for PA boundary conditions.

Objectives

- Assess simplifications used in PA models.
- Assess the constraining power of tracer experiments for PA models.
- Provide input for site characterisation programs from a PA perspective (i.e., provide support for site characterisation program design and execution aimed at delivering needed data for PA).
- Understand the site-specific flow and transport behaviour at different scales using SC models.

Framework and proposed site

SC and PA models are applied to two spatial scales:

- Single fracture scale (TRUE-1 site)
- Fracture network (block) scale

and two temporal scales:

- Traditional tracer experiment (SC time scale)
- PA time scale prediction

Framework and proposed site (cont.)

Observe:

- Fracture network (block) scale: a synthetic block based on the Prototype Repository, TRUE Block Scale, TRUE-1 and FCC features.
- Transport is considered from a virtual canister emplacement location in the Äspö HRL rock mass to a structural feature at a specified distance (starting from a few meters to 50-100 m).
- The addressed scale may be extended to site scale (canister to biosphere). For this option, geochemical data may also be utilised similar to Task 5.

Scope

- **Task 6A:** Model and reproduce selected TRUE-1 tests with a PA model and/or a SC model.
- **Task 6B:** Model selected PA cases at the TRUE-1 site with new PA relevant boundary conditions and temporal scales.
- **Task 6C:** Develop a 50-100m block scale synthesised structural model.
- **Task 6D:** Using the synthetic structural model, a TRUE-Block Scale type tracer experiment is modelled.
- **Task 6E:** Using the synthetic structural model, a reference set of PA time scales and boundary conditions are modelled.

Organisation

- Hierarchical structure:

Task Force ->Project Manager ->Technical Lead ->
Project Technical Teams

Task Force ->Technical Reviewers

- Project manager responsible for co-ordination of project.
- Technical lead responsible for development of project data base, structural framework, assumptions, benchmark cases, etc.

Time Schedule

- Project Initiation / TF#14 November 2000
- Present preliminary SC and PA simulation results for Tasks 6A and 6B / TF#15 Aug 2001
- Define Task 6C structural-hydraulic model based on suggestion produced prior to workshop / Workshop with TF#15 Aug 2001
- Present final results for Tasks 6A and 6B, and preliminary results for Task 6D / TF#16 April 2002
- Present final results for Task 6D and preliminary results for Task 6E / TF#17 November 2002

Time Schedule (cont.)

- Present final results from Task 6E / TF#18 July 2003
- Workshop for definition of site characterisation requirements according to preliminary results / Workshop with TF#18 July 2003
- Present final Task 6D/E sensitivity studies / TF#19 March 2004
- Complete preliminary reporting and preliminary review results / TF#19 March 2004
- Final Reporting and Evaluation of Task 6 / TF#20 December 2004

Detailed Suggestions

- Project sequence should be followed and documented to ensure that all models develop in a consistent, logical, and comparable fashion.
- Modellers are encouraged to provide the adopted performance measures for models with varying degrees of simplification in order to quantitatively demonstrate the rationale for simplifications.
- The task should employ a PA time scale, i.e. ten thousand to one million years (Task 6B and 6E).

Detailed Suggestions (cont.)

- Common boundary conditions should be set by the Task 6 project team.
- The horizontal distance from canister to closest important fracture zones should be on the order of 50 to 100 meters.
- A limited group of radionuclides with a range of half-lives and sorption parameters (Cs, I, Th, Se) should be used in the simulations.
- Injection mode will be selected by the Task 6 project team. Injection should take place during a long enough time interval to ensure matrix diffusion effects (Task 6B and 6E).

Detailed Suggestions (cont. 2)

- Modelling groups can develop the SC and/or PA-type models to the level of geological, hydrogeological, geochemical, and transport detail they feel is appropriate for the tasks.
- No treatment of engineered barriers and the disturbed zones.
- Reference cases (Task 6A and 6D) need to be defined in sufficient detail such that groups could in theory produce at least one identical result.

Performance Measures/Output

- Cumulative release (Bq/yr) to the fracture zone at the downstream boundary (e.g., time to peak or specified regulatory time).
- Magnitude of peak release (Bq/yr) and time to peak release.
- Retention ratio [%].

Also

- Sensitivity studies of alternative geological assumptions.
- Measures of the flow field (FWS/Q), f(tau) .

Expected Final Products

- Guidance for site characterisation requirements.
- Increased confidence in the simplifications and assumptions used in PA flow and transport approaches.
- Demonstration of rationale for abstraction process when going from SC to PA models.
- Statements on differences between SC and PA models.
- Improved understanding of flow and transport at PA scales based on studies using Äspö data.
- Visualisation of flow and radionuclide transport pathways and processes.

Appendix H

Task 6 proposal

M Uchida (JNC)

Task-6 Proposal
-Performance Assessment Modelling Using Site Characterisation Data (PASC) -

Task-6 Working Group:

J-O. Selroos, M. Uchida, H. Benabderrahmane, A. Winberg, I. Rhén, W. Dershowitz

Issues

- Transport from canister to site scale feature ($T>10^{-5} m^2/s$) (commonly up to 50-100m) is a critical for retardation to many countries.
- Single fracture → Fracture network in this scale is of primary importance

- Necessity to fill a gap between SC and PA
- Value of in-situ tracer experiment has been argued for long time (Geotrap WS#1, 1996) yet no concrete conclusion is obtained.
- In-situ tracer experiment is commonly dominated by faster processes which are sometimes not relevant to PA. (Even non-conservative De)
- There is a need to clarify important structure/processes which is more relevant to PA.
- This could provide a guide to SC data acquisition.

- Necessity to build confidence in simplification
- Simplification needs to be justified and uncertainty should be quantified.
- This can be achieved by applying models with various level of simplification to the same problem.

Objectives

- **Site Charactersation**
- **Understand how much the in-situ tracer experiment can constrain PA.**
- **Identify further data need from PA. → Provide guidance to SC.**
- **Understand site specific flow and transport behaviors through modeling.**

- **Performance Assessment**
- **Identify important processes/structure for long-term prediction.**
- **Build confidence in simplification by quantifying associated uncertainty**
- **Provide a benchmark for model comparison**

How Task-6 Tries To Answer Issues

- Apply both SC BC's and PA BC's in time and scale.
  → Two meanings:
  1. Determine which structures/processes is important for SC or PA.
  2. Study impact of different flow geometry on parameters
     → How anisotropic heterogeneity affects F-factor, when different flow field is used (RC/DP for SC, Parallel for PA.)

- Honor the actual field tracer experiment and add PA assumptions at later stage

- Start from simple to complicated system:
  → Single fracture → Fracture network

- Apply various levels of simplification and quantify uncertainty.
  → Two simplifications:
  1. Detailed structure → Simplify geometry + modify parameters (such as α)
  2. Processes → Approximate with other process model + modify

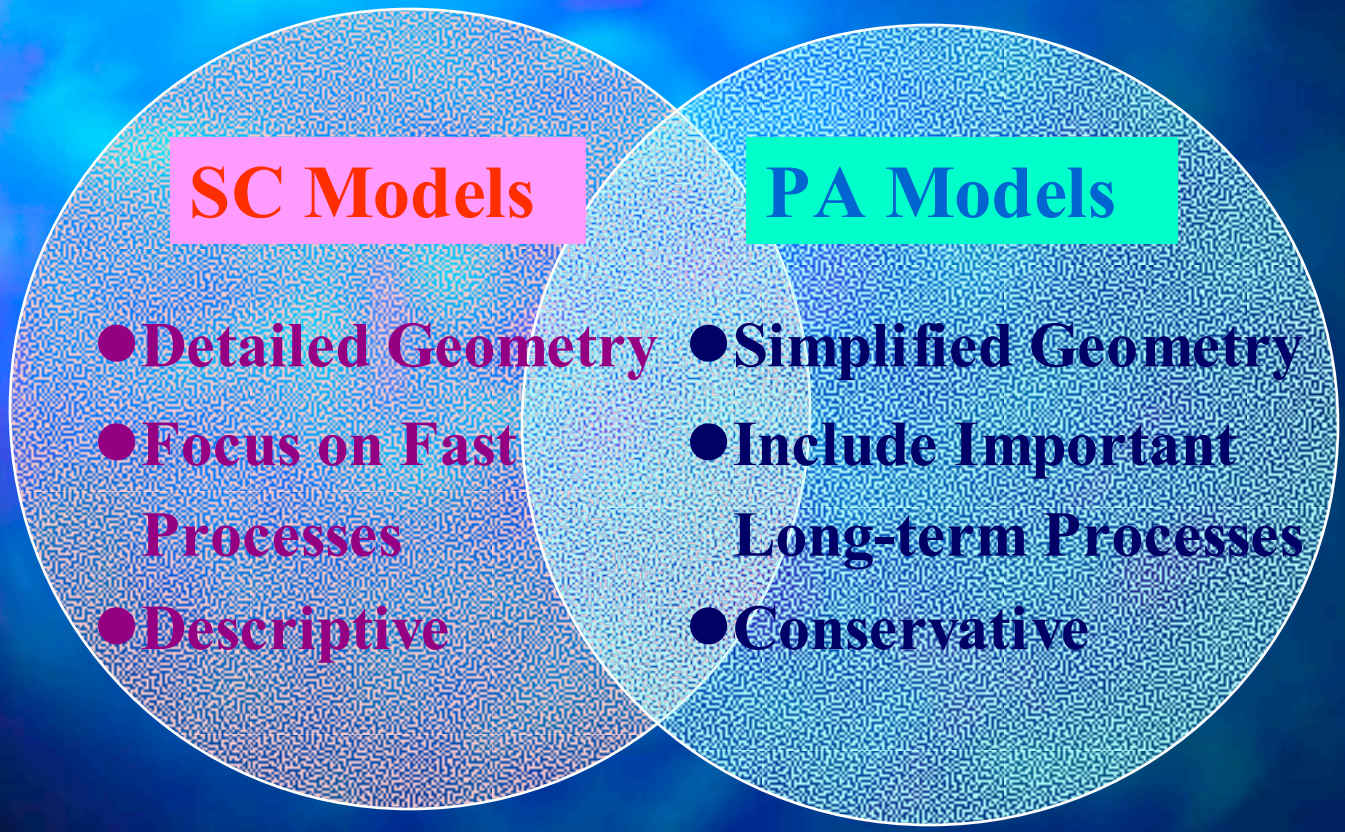
Remarks on SC models and PA models

- 3 kinds of models (Tsang, C. 1994; GEOVAL '94)
  - Single Process Model → Can be compared with laboratory experiment.

  - Research Model → Can be compared with more complicated experiment
    → More descriptive in heterogeneity and processes
    → Stronger link to measurement
    → Equivalent to SC model.

  - Long-term Predictive Model
    → Can be applied to long-term predictions.
    → General simplification in geometry
    → Includes important processes to long-term prediction
    → Equivalent to PA model.
    → Can be applied to in-situ tracer experiment when streamlines are provided by flow model

Remarks on SC models and PA models



PA Models can be used to explain in-situ tracer experiment when combined with flow model

The Role of Each Subtask in Task-6

Sub task	Structure	BC's, Time	Flow Field	Objectives
6A	Single Fracture (TRUE-1)	SC	RC/DP	1. Provide basis for further comparison 2. Study constraining power of tracer test.
6B	Single Fracture (TRUE-1)	PA	Parallel	1. Study how uncertainty increase due to simplification 2. Identify important assumption
6D	Fracture Network (TRUE BS + Other)	SC	RC/DP	1. Provide basis for further comparison 2. Study constraining power of tracer test.
6E	Fracture Network (TRUE BS + Other)	PA	Parallel	1. Study how uncertainty increase due to simplification 2. Identify important assumption in network scale by sensitivity studies

Remarks on SC models and PA models(2)

- Better way to say SC and PA models are degree of detail in structure/processes in model
- Structure

Finest → include microstructure, multi-layers, gouge
→ Limited data available for Feature A.
→ Use Martin Mazurek's study on microstructure of similar fracture or generic assumption but <u>honor the experiment</u>.
→ 1D bundles (PSI), pipe network, 3D

Moderate → In-plane heterogeneity of K field

Remark: Desirable to avoid tracer experiment in multiple fractures in Task-6A,B.

Possible Difficulty in Task-6

- Need to make assumptions where data are not available.
- This task is a brain exercise rather than matching data
  → Needs your experience and imagination on PA perspective
- Key is "Honor the data" and make reasonable assumption where data is not available
- Another way to call this exercise is *"Uncertainty Assessment Study at the stage of having a set of in-situ tracer experiments"*

Sharing Efforts in Task-6

- Modeling Teams can address any issues relate to geosphere retardation

- Modeling team should consider which FEPs are important and address their consequence as quantitatively as possible within reasonable range of assumptions.

- Focus on solute transport is recommended because tracer experiments are not originally designed for other purposes.

  → Given freedom

  1. Detail of microscale geometries
  2. Alternative processes for Adevection-Dispersion-Sorption-Matrix Diffusion

Appendix I

Example Task 6 simulation

B Dershowitz (Golder)

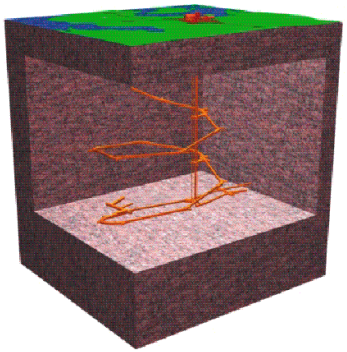
Example Task 6 Simulation
Cs-135 Transport in Feature A

Bill Dershowitz [2], Masahiro Uchida [1],

Göteborg, November 2000

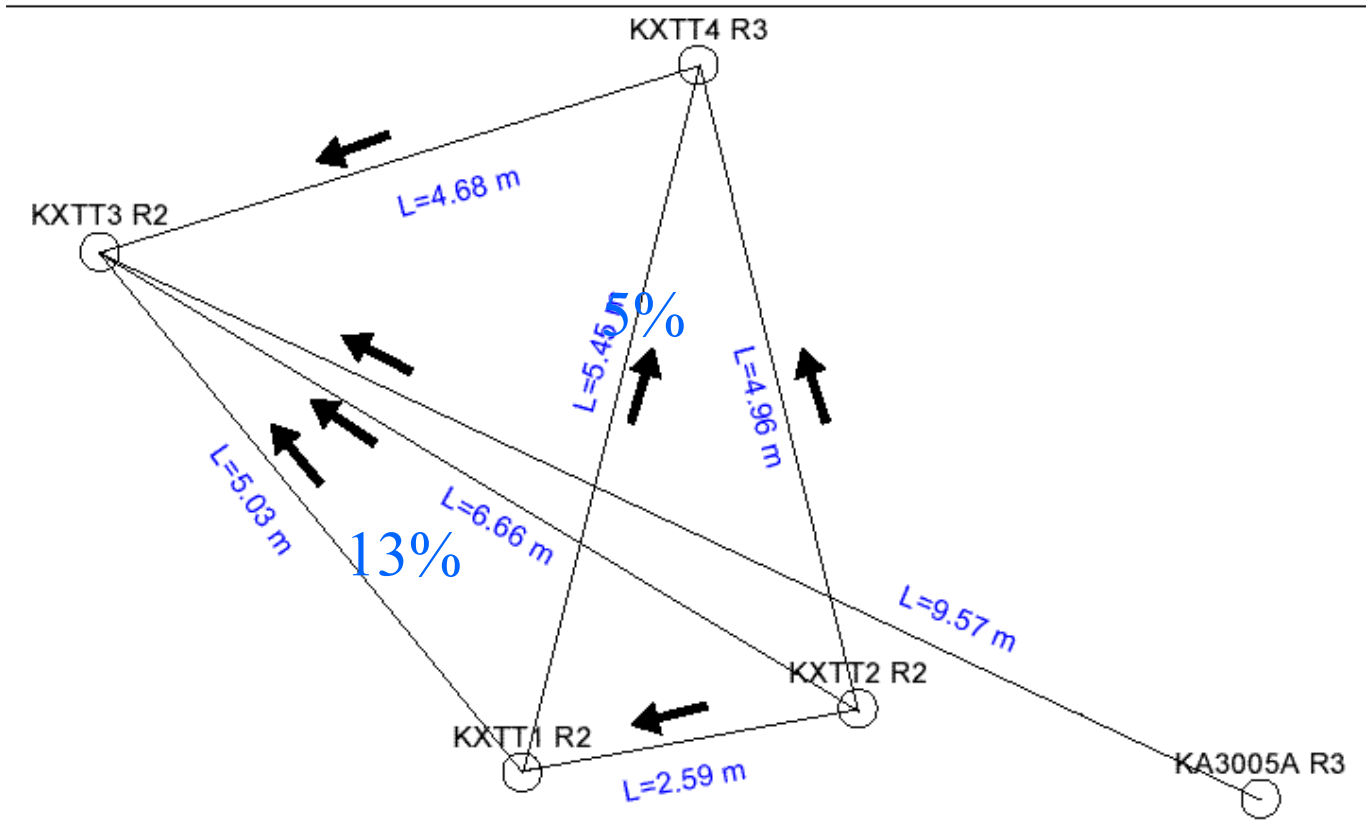
1. Japan Nuclear Fuel Cycle Development Corporation,

2. Golder Associates Inc



JNC サイクル機構

Feature A Transport Pathways

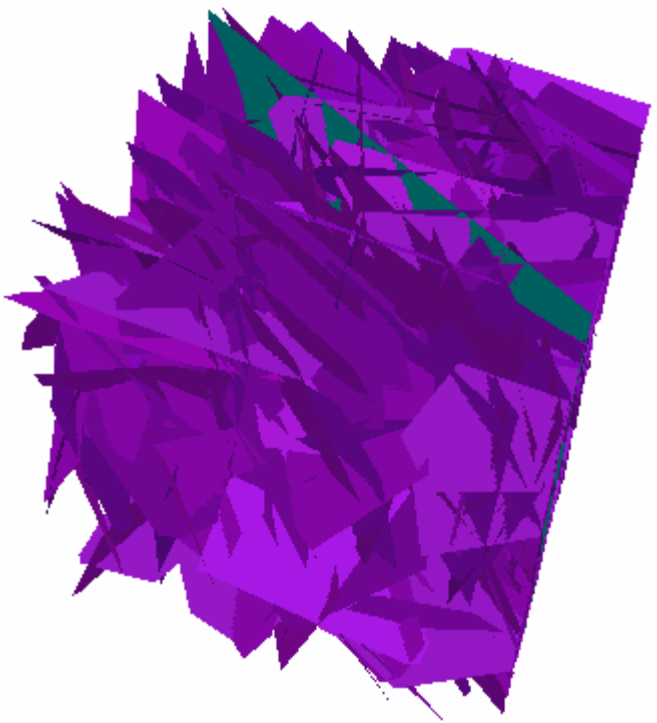


JNC サイクル機構

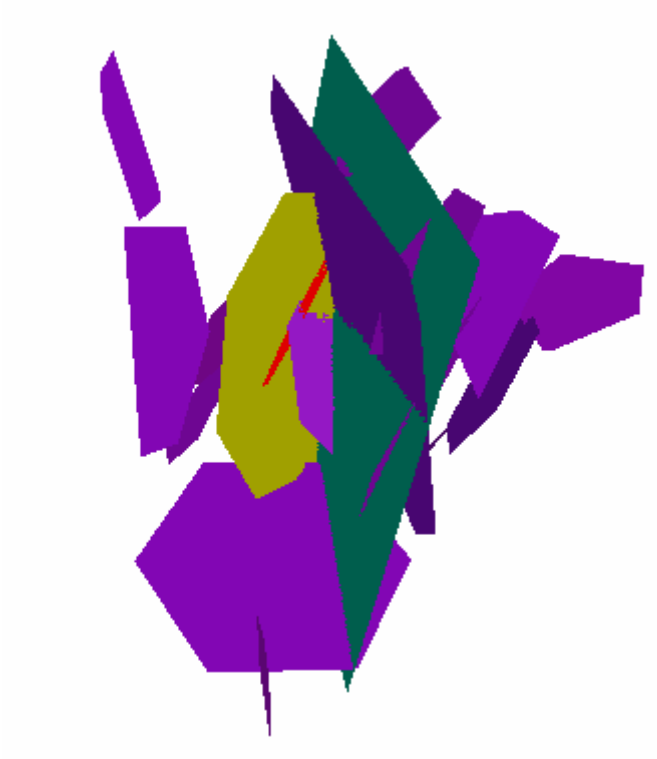
3D DFN Model

- **Features NW, A, and A' and background fractures**

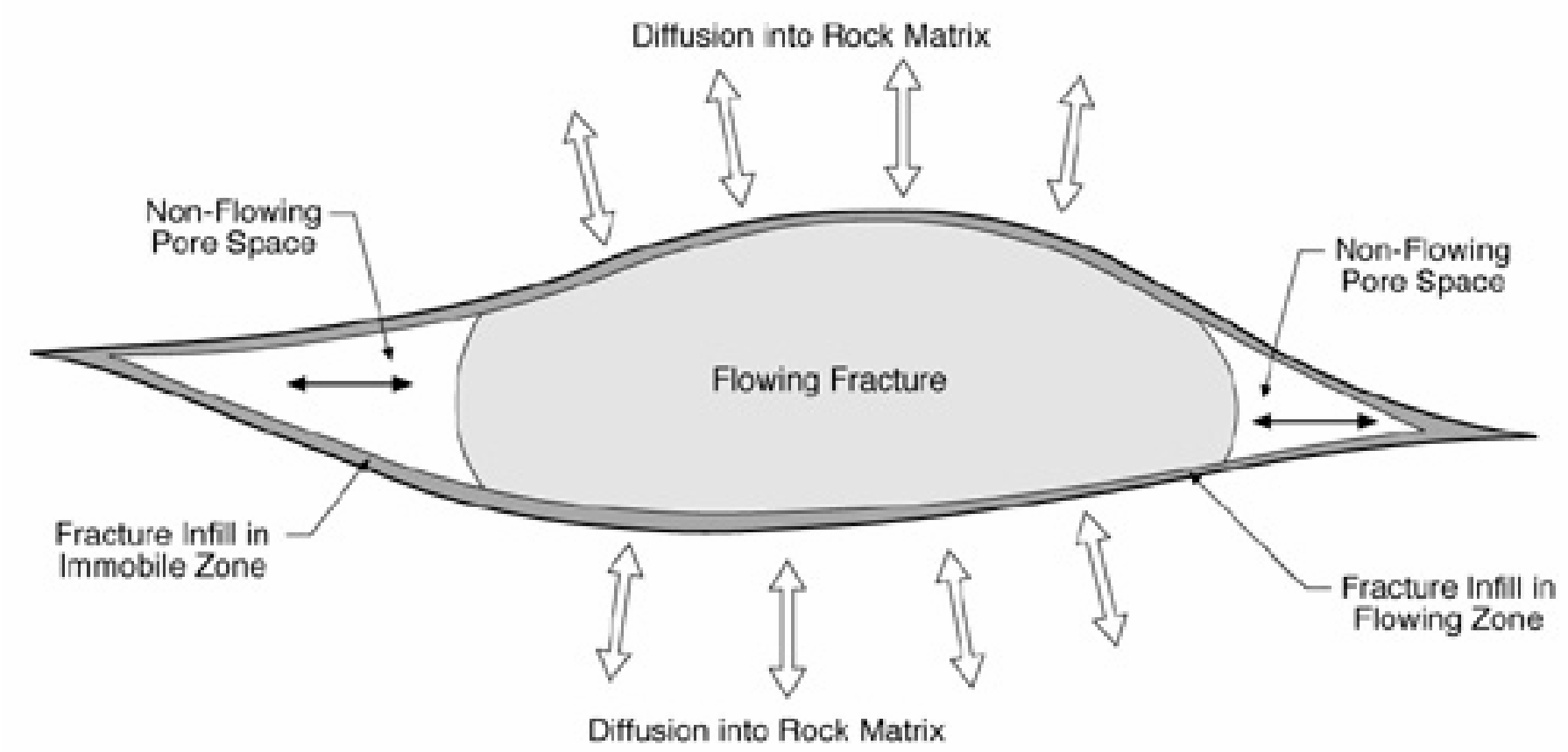
All 359 background fractures



5% background fractures

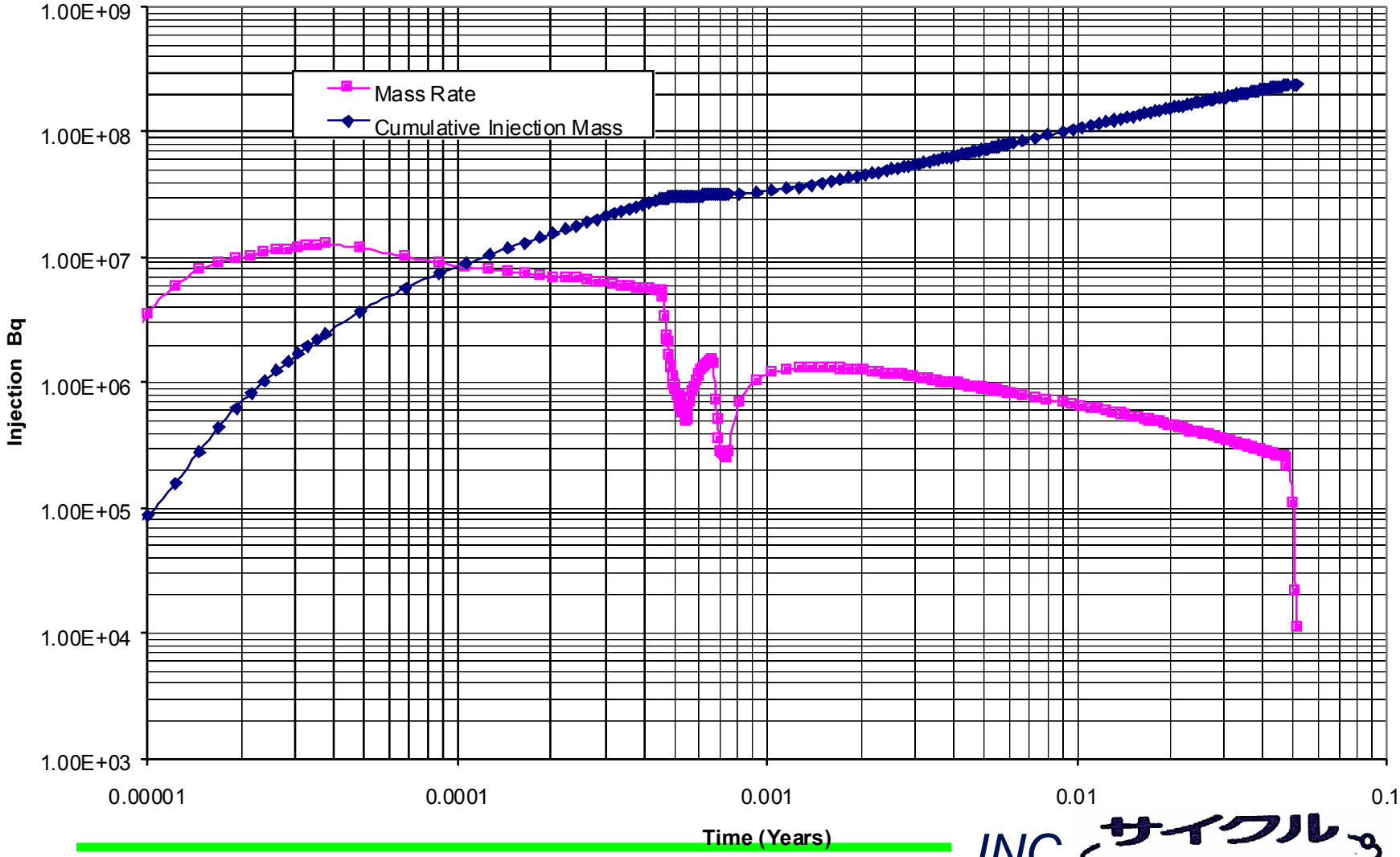


Mobile/Immobile Zone Transport
JNC/Golder FracMan/PAWorks Concept



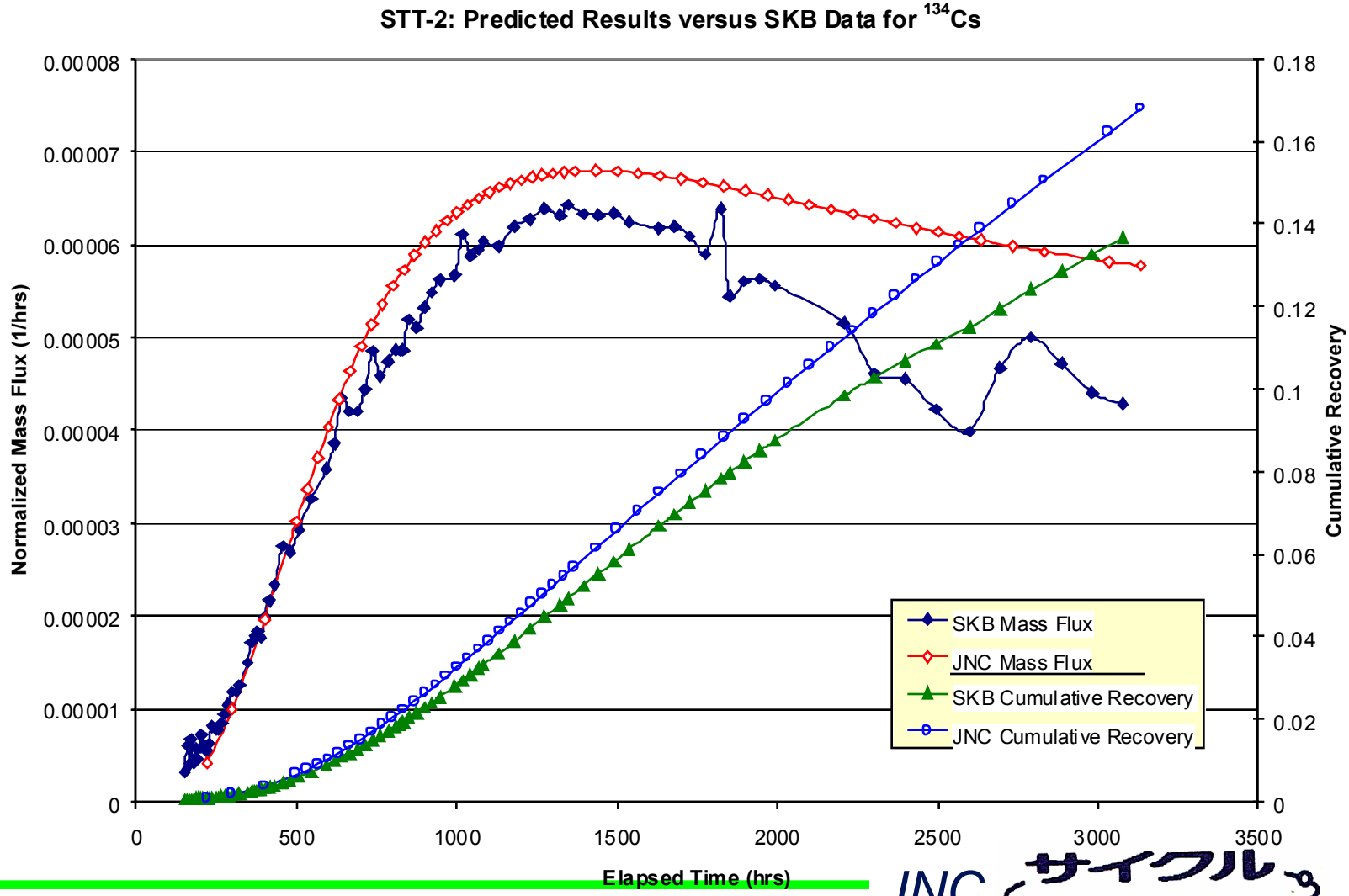
JNC サイクル機構

STT-2 Cesium
Injection Time History



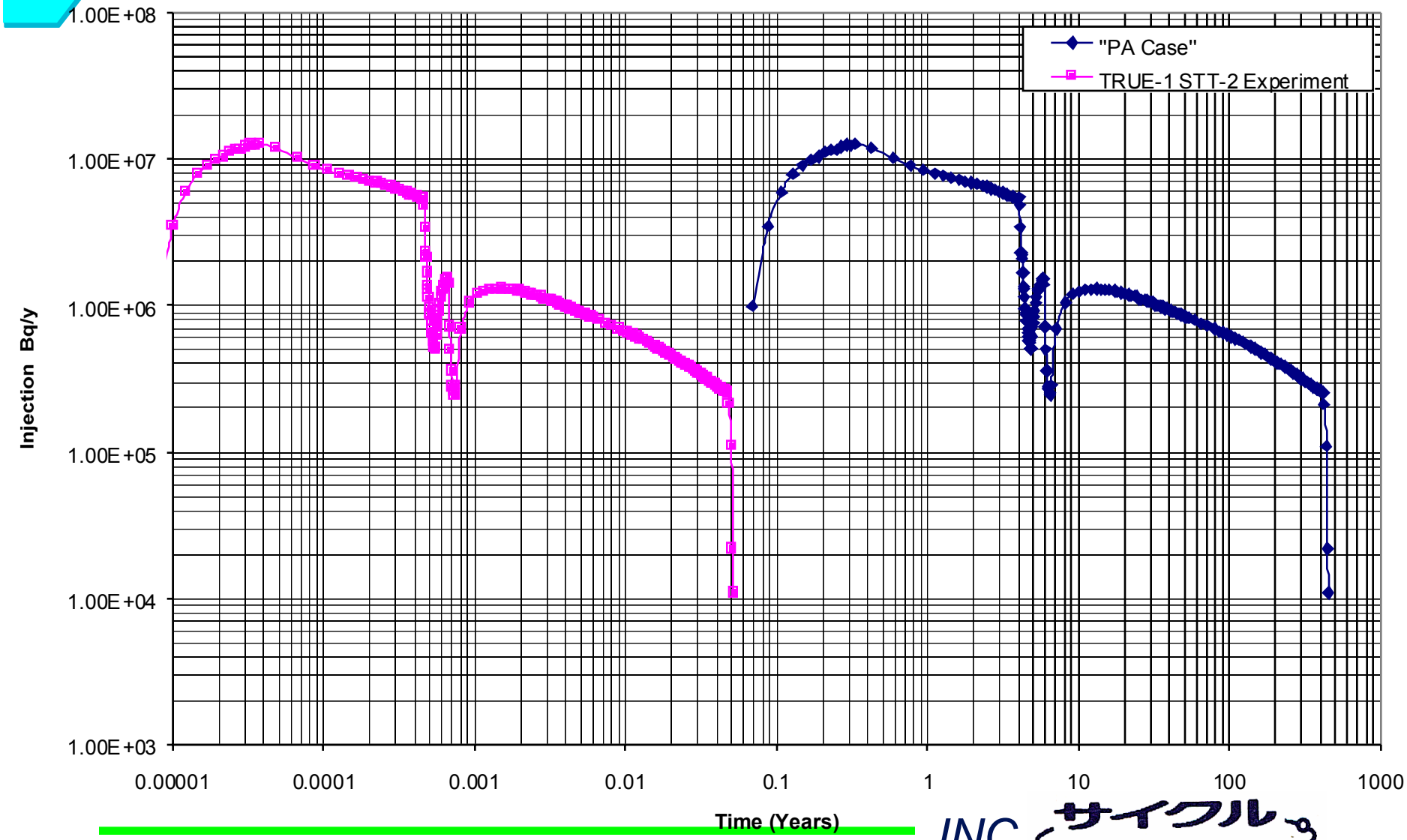
JNC サイクル機構

STT-2 Cesium
Recovery Predicted within 3%



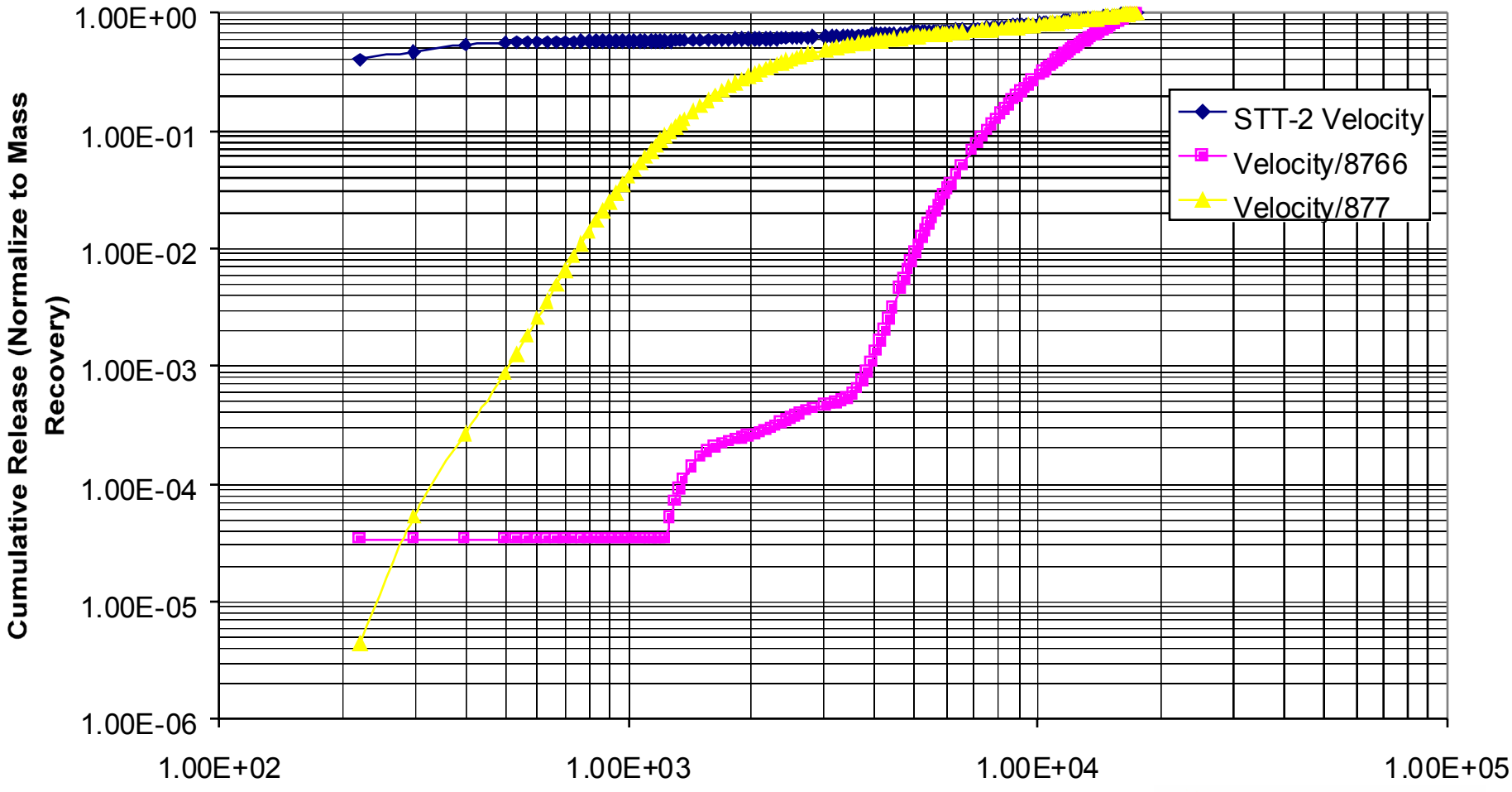
JNC サイクル機構

Task 6 “PA” Source and Recovery Cesium



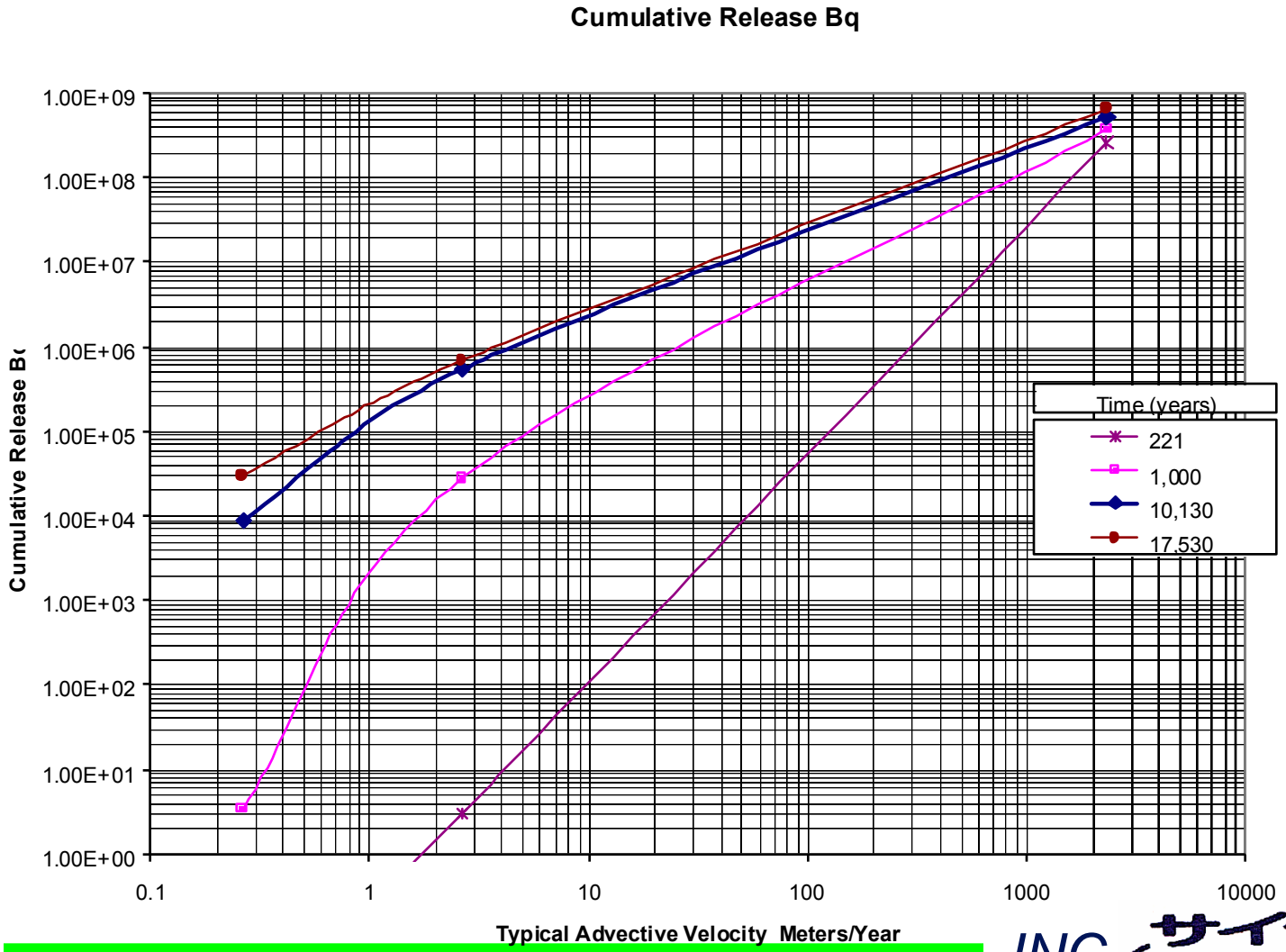
JNC サイクル機構

Normalized Breakthrough Cesium-135



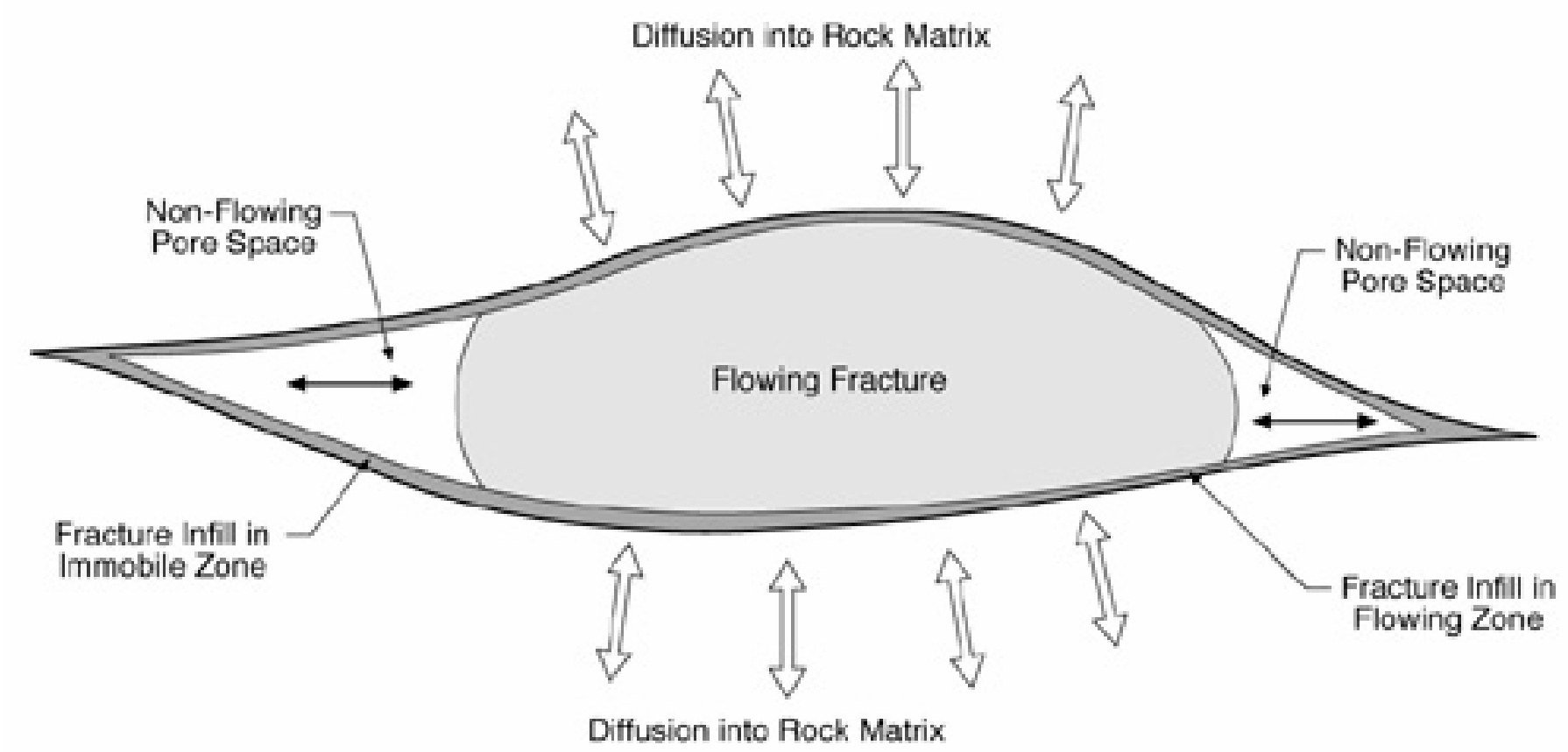
JNC サイクル機構

Cumulative Release Cesium-135



JNC サイクル機構

Mobile/Immobile Zone Transport
JNC/Golder FracMan/PAWorks Concept

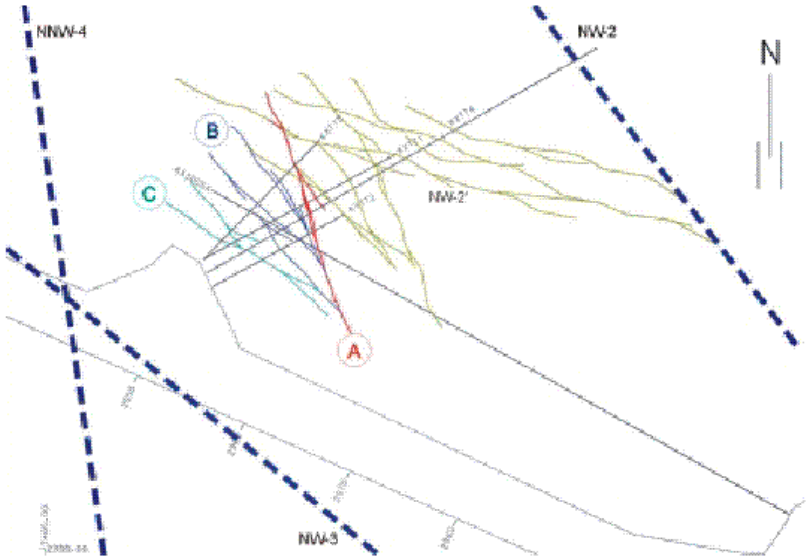


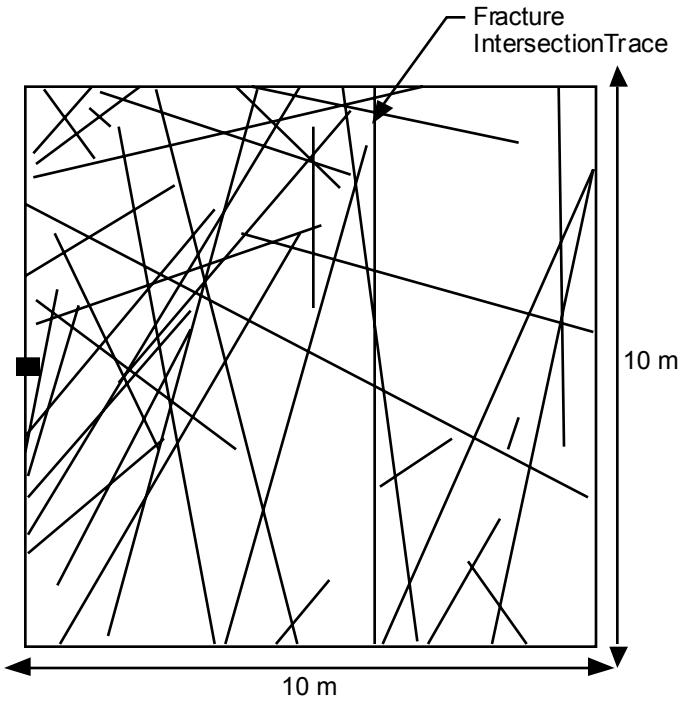
JNC サイクル機構

Conclusions

- Task 6 Potentially Provides a Link Between PA and Site Characterization Codes
- Task 6 Potentially Supports Extension of Site Characterization Experiments to PA Time and Space Scales
- Task 6 Potentially Provides Guidance for Prioritization of Site Characterization

Conductive Fractures Intersecting “Feature A”





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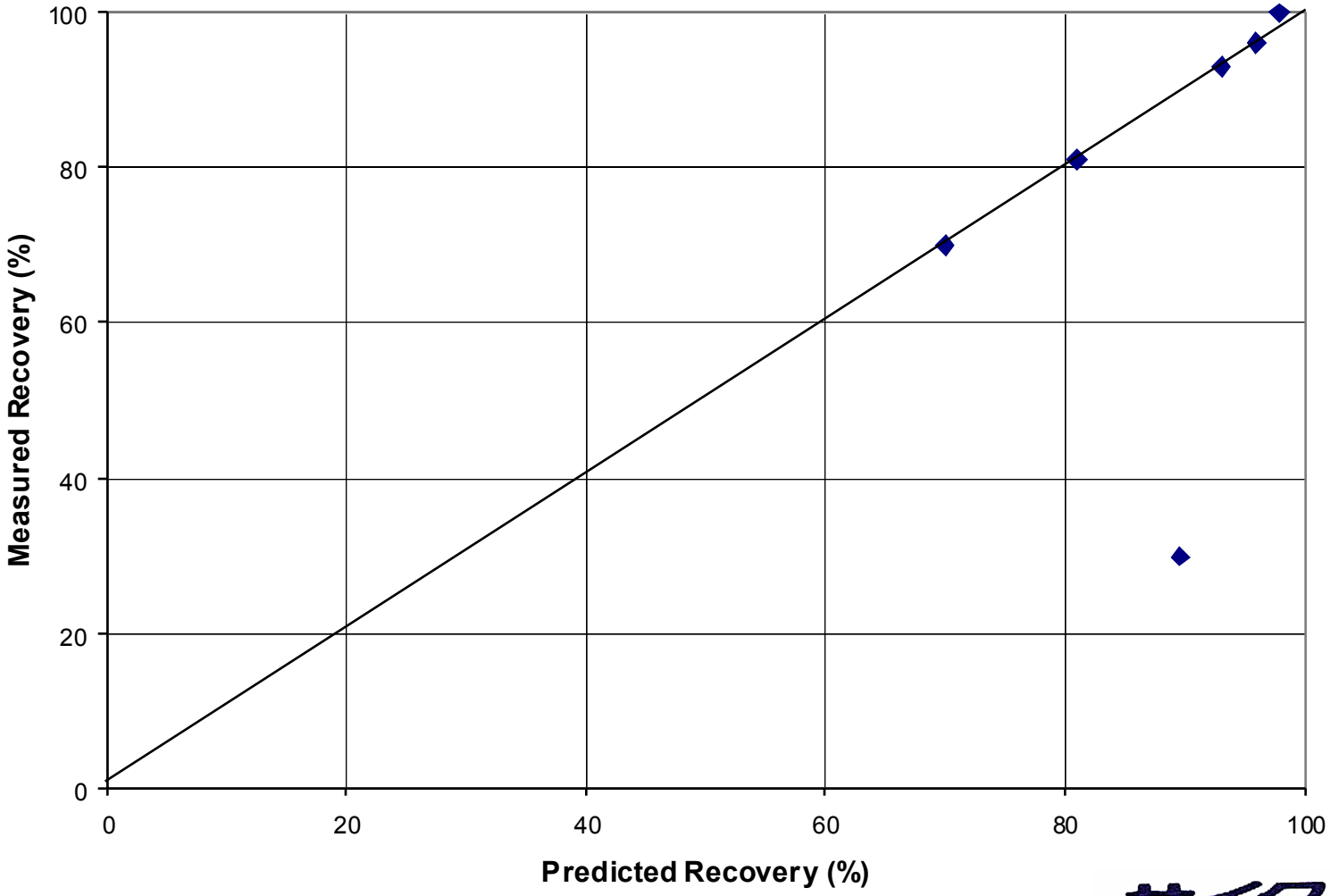
Performance of STT-1b recovery predictions



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JNC/Golder Prediction of STT-2
29 of 40 predictions within 20%

	Comparison of **Prediction** against *Measurement*			
Tracer	***t5 (h)***	***t50 (h)***	***t95 (h)***	***% Recovery***
Uranin	★ 9.7 *10.58*	★ 65.3 *69.50*	★ 247.9 *329.42*	★ 100 *110.8*
HTO	★ 11.3 *12.50*	61.3 *79.83*	★ 229.5 *n/a*	★ 100 *90.0*
Na-22	★ 16.3 *16.00*	★ 105.3 *93.83*	★ 650 *n/a*	★ 100 *88.4*
Ca-47	★ 18.7 *23.00*	414.5 *126.83*	★ n/a *346.58*	50.7 *109.13*
Br-82	★ 9.4 *11.00*	135.3 *70.83*	★ n/a *n/a*	57.1 *91.96*
Sr-85	★ 22.7 *28.00*	★ 170.6 *157.83*	★ n/a *n/a*	★ 89.6 *85.64*
Ba-131	162.7 *76.83*	★ 1130.7 *736.83*	★ n/a *n/a*	18.3 *61.17*
Ba-133	180.1 *73.83*	★ 1106.6 *712.83*	★ n/a *n/a*	★ 76.1 *72.38*
Rb-86	n/a *126.83*	n/a *1129.33*	★ **n/a** *n/a*	0 *54.28*
Cs-134	★ 533.5 *1345.33*	★ n/a *n/a*	★ n/a *n/a*	★ 8.3 *13.66*

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