INTRACOIN

International Nuclide Transport Code

Intercomparison Study

FINAL REPORT LEVEL 1

Code verification

COLUMN
DRAMA
DPCT
FTRANS
GARD2S
GEOS
GETOUT
METIS
MMT
NUCDF
NUTRAN
NWFT/DVM
PORFLO
RANCH
RANCHN
SWENT
SWIFT
SWIFT II
TRANSAT
TROUGH
TRUCHN
UCB-NE

September 1984
INTRACOIN
LEVEL ONE
REPORT

International Nuclide Transport Code Intercomparison Study
PREFACE

An international cooperation project, INTRACOIN, for comparing models for transport of radioactive nuclides in geologic media was initiated at a meeting in Stockholm, June 17-18, 1981. The following organisations have participated in the study:

Atomic Energy of Canada Ltd
Commissariat à l’Energie Atomique/
Institut de Protection et de Sécurité Nucléaire
Nationale Genossenschaft für die Lagerung Radioaktiver Abfälle
National Radiological Protection Board
Projekt Sicherheitsstudien Entsorgung
Technical Research Centre of Finland
Swedish Nuclear Fuel Supply Co
Swedish Nuclear Power Inspectorate
U.K. Atomic Energy Authority/
Atomic Energy Research Establishment
U.S. Department of Energy
U.S. Nuclear Regulatory Commission

CANADA
FRANCE
SWITZERLAND
UNITED KINGDOM
FEDERAL REPUBLIC OF GERMANY
FINLAND
SWEDEN
SWEDEN
UNITED KINGDOM
USA
USA

This is a report of the first phase of the project which was devoted to a comparison of the numerical accuracy of the computer codes used in the study. Later phases are the subject of a separate report. This report was prepared by the project secretariat and published after approval by the coordinating group. Neither the coordinating group nor the project secretariat take any legal responsibility for the results presented in this report or their use.
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Appendix 2  Model and code characterizations

Appendix 3  Results from level 1
INTRODUCTION

1. BACKGROUND

The safe handling and disposal of radioactive wastes is a prerequisite for the exploitation of nuclear power. Extensive research and development in the field of management and disposal of radioactive waste is conducted in many countries. To a large extent this work is directed to the finding of methods for the disposal of high-level waste including spent nuclear fuel if regarded as waste.

The disposal of high-level waste in deep geological media is a method of disposal that is being evaluated in several countries. For such evaluations it is necessary to have adequate data on the characteristics of the different sites and the different repository designs. It is also essential to have appropriate tools for the evaluation of the safety of the disposal system.

An important part of the safety analysis of repository concepts is an assessment of release and transport of long-lived radioactive nuclides from the repository to the biological environment. In this assessment mathematical models describing the mechanisms involved in the nuclide transport from the repository to the biosphere are essential tools.

To improve the understanding of various strategies for radionuclide transport modelling an international cooperation project was set up with the participation of a number of organisations. In the project, INTRACOIN (International Nuclide TRAnsport COde INtercomparison study), a comparison between different computational codes describing transport of radionuclides in geologic media is made.

1.2 OBJECTIVES

The purpose of the project is to obtain improved knowledge of the influence of various strategies for radionuclide transport modelling for the safety assessment of final repositories for nuclear waste. According to the objectives formulated when the project was founded the work should deal with:

a) the impact on the transport calculations of incorporating various physico-chemical phenomena;

b) the impact of choosing different solution algorithms;

c) the closeness of fit of different models to in-situ measurements.
1.3 PROJECT ORGANISATION

The organisation of the INTRACOIN study is regulated in an agreement between the participating organisations (Parties). According to the agreement the study is directed by a coordinating group consisting of one representative from each Party. The Swedish Nuclear Power Inspectorate (SKI) acts as managing participant. Each Party organises one or several project teams which performs the calculations defined by the coordinating group and formulated in detail by the project secretariate.

The project secretariate has been set up by SKI in cooperation with the Swiss organisation NAGRA. The Swedish company KEMAKTA Consultants Co. acts as principal investigator for the study and performs the technical work within the project secretariate in cooperation with the Swiss Federal Institute for Reactor Research (EIR).

Each Party covers the costs for its participation in the study and is responsible for organising the budget for its own project team or teams. The administrative effort for the project secretariate is covered by SKI while the cost for the technical and scientific work within the secretariate is covered jointly by SKI and NAGRA according to a special agreement.

In Appendix 1 a survey of the project organisation as well as a list of the Parties setting up the INTRACOIN study, coordinating group members and project team leaders is given. The Appendix also contains a list of abbreviations used in this report for parties and project teams.

During the progress of the study workshops have been organised. These have offered good opportunities to discuss the results and for informal exchange of ideas among the participants. The advancement of the study is documented in a series of Progress Reports.

1.4 LEVEL STRUCTURE

The INTRACOIN code comparison is performed at three levels aimed at examining:

1) The numerical accuracy of the codes compared.
2) The capabilities of the codes to describe in-situ measurements.
3) The quantitative impact of various physical phenomena on the nuclide transport calculations in a typical repository scenario assessment.
In this report the level 1 results are presented.

At this level the numerical accuracies of the codes are compared. This has been achieved by comparing computational results from analytical solutions with results from numerical solution algorithms in such cases where this is possible, as well as by intercomparing results from codes using different numerical methods to solve the same problem. A more detailed description of the cases which have been calculated is found in Chapter 2.

1.5 PARTICIPATING CODES

The radionuclide transport codes that are compared in INTRACOIN can be divided into five groups:

1. One-dimensional advection-dispersion models.
2. One-dimensional advection-dispersion models with piecewise constant parameters.
4. Models including non-linear chemical effects.
5. Combined models including also equations for hydrology and heat transport.

The fifth group of models includes features that are beyond the scope of INTRACOIN to compare.

The codes participating at level 1 are listed in table 1.1 together with their main features. A more complete description of the codes and their underlying mathematical models can be found in Appendix 2.

1.6 STRUCTURE OF THE LEVEL 1 REPORT

In Chapter 2 a description is given of the work performed at level 1, including the definitions of calculated cases. These cases range from simple cases with one-dimensional transport with constant parameters to two-dimensional cases with or without matrix diffusion.

The results are presented in Chapter 3. Since the objective of level 1 is code verification the results are mainly presented as comparisons of calculations performed with different codes on identical cases with identical parameter values. For one of the cases a relatively large number of parameter variations have been calculated. These are presented as maximum concentrations as functions of the parameter values. Furthermore Chapter 3 contains a discussion on the impact of boundary conditions on the results.
<table>
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<th>Method of solution</th>
<th>Dimensionality</th>
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<td>Analytical</td>
<td>Depending on Application</td>
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</table>

1) Two GETOUT-versions called GETOUTO (ONWI) and GETOUTUV (VTT) participate. They differ in the treatment of daughter nuclides.

2) Two NMT-versions called NMTIDPUL (PHI) and NMTVTT (VTT) participate.

3) A separate program, CONERA, is used together with RANCFN to treat a source boundary condition.

4) X denotes a number that is different for the various UCB-codes.
The results are discussed in Chapter 4 where conclusions from the level 1 calculations are drawn and recommendations for future bench-mark studies are made.
DEFINITION OF LEVEL 1

2.1 GENERAL

The computational cases set up at level 1 were designed to test as many of the nuclide transport features of the models in the five groups described in section 1.5 as possible. To this end seven cases were defined at the first coordinating group meeting in Stockholm, June 17-18, 1981. The main features of the cases are described below:

1. One-dimensional advection-dispersion, constant migration parameters (ground water velocity, retention factors and dispersivity), and constant leach rate.

2. One-dimensional advection-dispersion in a layered medium (piece-wise constant migration parameters).

3. One-dimensional advection-dispersion with continuously varying parameters.

4. Two-dimensional advection-dispersion with constant retention factors and dispersivity.
   a) Parallel flow field and radial dispersion
   b) Two-dimensional flow field and radial dispersion.

5. One-dimensional advection-dispersion with diffusion into the rock matrix.

   a) Parallel flow field and radial dispersion
   b) Two-dimensional flow field and radial dispersion.

7. One-dimensional advection-dispersion with linear mass transfer kinetics and constant migration parameters.

The cases 1 and 3 are tailored to test models from group 1 while case 2 is designed for models from group 2. In addition case 1 serves as a common case to be solved with all models. The cases 5 and 6 are defined as a test for models in group 3 and case no. 7 is designed for testing the fourth model group. As the models in the groups 3, 4 and 5 very often are capable of handling multidimensional problems it was decided to include case 4. The cases only include a test of the radionuclide transport part of the models in group 5. Neither was a three-dimensional case included because too few of the participating codes are able to treat such problems.
The cases computed by the different project teams are given in Table 2.1. The project teams are listed in alphabetical order following the INTRACOIN Party responsible for organising the calculations. The names of the codes used have been listed together with the project teams. Descriptions of these codes can be found in Appendix 2. The names of the Parties and the names of the project teams have been abbreviated. The abbreviations used are explained at the end of Appendix 1.

In case 1 a number of parameter variations have been defined (see section 2.2.2). One of these is called the basic set and has been calculated with almost all of the participating codes allowing for a comprehensive intercomparison.

It should be emphasized that the parameter values at level 1 were chosen to give a sensitive comparison of the codes. The values chosen are therefore in some cases clearly unrealistic with respect to safety analyses whereas the realism of other values can be disputed.

2.2 DEFINITION OF LEVEL 1 CASES

2.2.1 General

The definitions of the seven cases at level 1 are given in section 2.2.2. This section uses a short-hand notation for parameter values which is also used in the presentation of results. The parameters are defined by a letter and a digit identifying the parameter and its value respectively. The following letters are used for identifying parameters:

B Inlet boundary condition
E Exit boundary condition
I Nuclide inventory (activity units)
L Migration path length (m)
P Peclet number (migration length/dispersion length)
R Retention factors
T Leach duration (yrs)
V Ground water velocity (m/yr)

Two radionuclide decay chains have been used (denoted I₁ and I₂), both with three chain members. The chain I₁ is U-234 → Th-230 → Ra-226 and the chain I₂ is Cm-245 → Np-237 → U-233. These have been combined with two sets of retention factors out of which the set R₁ contains larger retention factors than R₂.
Table 2.1. List of bench-mark cases at level 1 computed by the various project teams.

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<td>EIR</td>
<td>CONZRA/RANCH</td>
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<td>X</td>
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<td>KTH</td>
<td>TRUCIHN</td>
<td>X 8)</td>
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<td></td>
<td></td>
<td>NUCDIF</td>
<td></td>
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<tr>
<td>SKI</td>
<td>Kemakta</td>
<td>COLUMN</td>
<td>X</td>
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<td>Intera</td>
<td>FTRANS</td>
<td>X</td>
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<td></td>
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<td>X</td>
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<td>GETOUT</td>
<td>X</td>
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</tr>
<tr>
<td></td>
<td></td>
<td>MMTVTT</td>
<td>X</td>
</tr>
</tbody>
</table>

1) Abbreviations used for project teams and Parties are explained in Appendix 1.
2) The codes are described in Appendix 2.
3) Axial dispersion omitted.
4) Dispersion omitted.
5) Chain decay and dispersion omitted.
6) The results of cases 4b and 6 are not discussed in this report because too few results were submitted to give a sensible comparison.
7) Two-layer calculations.
8) Retention calculated with matrix diffusion.
Two alternative inlet boundary conditions were defined where $B_1$ is a concentration boundary and $B_2$ is an injection rate boundary. Two interpretations of the boundary condition $B_2$ are represented in the results (see also Chapter 3). Some of the project teams have thus used a source in an infinite space whereas the rest of the teams have used a flux across a finite boundary to the modelled domain.

The exit boundary conditions were not originally defined. However, the project teams have used three exit boundary conditions according to the following definitions:

$E_1$ A semi-infinite boundary condition, i.e. the concentration approaches zero when the migration length approaches infinity.

$E_2$ The concentration equals zero outside the boundary. This condition is not the usual zero concentration boundary condition.a)

$E_3$ The concentration gradient equals zero on the boundary (pure convective flux)a).

The above means that the complete calculation of a case involves typically 4 combinations of inventories and retardation factors plus eventual variations of the boundary conditions. In addition for the first case, most of the parameters have been given alternative values.

2.2.2 Case definitions

Case 1

Case one is a one-dimensional transport case with constant parameters. It includes a basic set of parameter values and a number of parameter variations.

The basic set of parameter values includes two sets of retention factors and two independent decay chains. This means two or four runs depending on whether a code can handle several chains in one single run or not. Furthermore those project teams that can handle both a concentration boundary condition and an injection rate boundary condition have been requested to perform both calculations.

a) See Notes, (page 45)
The parameter variations are named by the letter indicating the parameter with a digit subscript indicating the sequence number of the specific value. Thus $P_1$ is the identification of a parameter variation in which the Peclet number is assigned the value 1000 (see below). The parameter values included in the basic set is indicated with the text "BASIC SET".

I) Nuclide inventories (Ref. 1) $I_k(0)^b$ (arbitrary units of activity) at time zero normalised to the most long-lived chain member.

$I_1$: Long-lived parent nuclide

<table>
<thead>
<tr>
<th>Nuclide k</th>
<th>$t_{1/2}$ (Ref. 2) yr</th>
<th>$I_k(0)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{234}U$ 1</td>
<td>2.445 + 5</td>
<td>1.000</td>
</tr>
<tr>
<td>$^{230}Th$ 2</td>
<td>7.7 + 4</td>
<td>0.010</td>
</tr>
<tr>
<td>$^{226}Ra$ 3</td>
<td>1.600 + 3</td>
<td>0.004</td>
</tr>
</tbody>
</table>

$I_2$: Short-lived parent nuclide

<table>
<thead>
<tr>
<th>Nuclide k</th>
<th>$t_{1/2}$ (Ref. 2) yr</th>
<th>$I_k(0)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{245}Cm$ 1</td>
<td>8.500 E + 3</td>
<td>0.700</td>
</tr>
<tr>
<td>$^{237}Np$ 2</td>
<td>2.14 E + 6</td>
<td>1.000</td>
</tr>
<tr>
<td>$^{233}U$ 3</td>
<td>1.592 E + 5</td>
<td>0.004</td>
</tr>
</tbody>
</table>

T) Leach duration

$T_1$: $T = 10^3$ yr
$T_2$: $T = 10^5$ yr BASIC SET

B) Boundary Condition$^c$

$B_1$: Concentration boundary condition.

The concentration at the inlet is defined by

$$C_k(0,t) = \frac{I_k(t)}{v \in F}$$

b) and c) See Notes (page 45)
Note:

\( v \in F \) is the water flow at the inlet.

The parameters are fixed as follows:

\( e = 0.01 \)
\( F = 100 \, \text{m}^2 \)

**B2**: Source boundary condition

The injection rate at the repository is defined by

\[ F_k(t) = \frac{I_k(t)}{T} \]

L) Migration length \( L \)

\( L_1: L = 500 \, \text{m} \) \hspace{1cm} **BASIC SET**
\( L_2: L = 5000 \, \text{m} \)

V) Interstitial ground water velocity \( v \)

\( v = 1 \, \text{m/yr} \)

P) Peclet number \( Pe \) (see list of nomenclature for definition)

\( P_1: Pe = 1000 \) or \( d) \)
\( P_2: Pe = 10 \) \hspace{1cm} **BASIC SET**
\( P_3: Pe = 1 \)

R) Retention factors\(^c)\)

\( R_1: \)

<table>
<thead>
<tr>
<th>Element</th>
<th>( R )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cm</td>
<td>5000</td>
</tr>
<tr>
<td>Np</td>
<td>700</td>
</tr>
<tr>
<td>U</td>
<td>300</td>
</tr>
<tr>
<td>Th</td>
<td>20000</td>
</tr>
<tr>
<td>Ra</td>
<td>10000</td>
</tr>
</tbody>
</table>

\(^c), \, d) \) and \( e) \) See Notes (page 45)
Case 2

This case is in principle based on the basic set of parameter values from case 1. However, the migration path has been divided into three zones with different retention factors (see figure 2.1). This means that the project teams have been requested to do calculations with the nuclide inventories $I_1$ and $I_2$ with boundary conditions $B_1$ and/or $B_2$ (see description of case 1) and leach duration $T_2$ ($10^3$ yrs). The ground water velocity and Peclet number are 1 m/yr and 10 ($P_e$) respectively throughout the whole column. The data that differ between the three zones are:

1) Migration length

zone 1: 50 m
zone 2: 100 m
zone 3: 350 m

Figure 2.1. Variation of retention factors along the transport path in case 2. The relative R-values reflect the conditions for set $R_1$. 

f) and g) See Notes (page 45)
R) Retention factors

<table>
<thead>
<tr>
<th>Element</th>
<th>Zone 1</th>
<th>Zone 2</th>
<th>Zone 3</th>
<th>Zone 1</th>
<th>Zone 2</th>
<th>Zone 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cm</td>
<td>10 000</td>
<td>5 000</td>
<td>2 500</td>
<td>500</td>
<td>60</td>
<td>30</td>
</tr>
<tr>
<td>Np</td>
<td>1 400</td>
<td>700</td>
<td>350</td>
<td>700</td>
<td>200</td>
<td>100</td>
</tr>
<tr>
<td>U</td>
<td>600</td>
<td>300</td>
<td>150</td>
<td>300</td>
<td>60</td>
<td>30</td>
</tr>
<tr>
<td>Th</td>
<td>40 000</td>
<td>20 000</td>
<td>10 000</td>
<td>5 000</td>
<td>500</td>
<td>250</td>
</tr>
<tr>
<td>Ra</td>
<td>20 000</td>
<td>10 000</td>
<td>5 000</td>
<td>2 000</td>
<td>20</td>
<td>10</td>
</tr>
</tbody>
</table>

The project teams have been requested to do calculations with both retention factor sets.

Case 3

This case is designed to be as comparable to case 2 as possible. It is therefore based on the basic set of parameter values from case 1 but with continuously varying retention factors (see figure 2.2). This means that the project teams have been requested to use the following parameter values:

Figure 2.2. Variation of the retention factors in case 3. The relation between the R-value at the downstream and upstream end of the path is the same as for case 2 (compare figure 2.1).
Nuclide inventories: $I_1$ and $I_2$
Leach duration: $T_2$ (10$^5$ yrs)
Boundary condition: $B_1$ and/or $B_2$
Migration length: $L_1$ (500 m)
Ground water velocity: $V$ (1 m/yr)
Peclet number: $P_2$ (10)

R) Retention factors

The variation of the retention factors with distance is expressed in analytic form $R = G + H \cdot \frac{xh}{l}$

where the constants are given in the tables below for the two sets of retention factors for which calculations have been made.

### R$_1$

<table>
<thead>
<tr>
<th>Element</th>
<th>$G$</th>
<th>$H$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cm</td>
<td>10 000</td>
<td>-7 500</td>
</tr>
<tr>
<td>Np</td>
<td>1 400</td>
<td>-1 050</td>
</tr>
<tr>
<td>U</td>
<td>600</td>
<td>-450</td>
</tr>
<tr>
<td>Th</td>
<td>40 000</td>
<td>-30 000</td>
</tr>
<tr>
<td>Ra</td>
<td>20 000</td>
<td>-15 000</td>
</tr>
</tbody>
</table>

### R$_2$

<table>
<thead>
<tr>
<th>Element</th>
<th>$G$</th>
<th>$H$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cm</td>
<td>500</td>
<td>-470</td>
</tr>
<tr>
<td>Np</td>
<td>700</td>
<td>-600</td>
</tr>
<tr>
<td>U</td>
<td>300</td>
<td>-270</td>
</tr>
<tr>
<td>Th</td>
<td>5 000</td>
<td>-4 750</td>
</tr>
<tr>
<td>Ra</td>
<td>2 000</td>
<td>-1 990</td>
</tr>
</tbody>
</table>

Case 4a

This case is based on the basic set of parameter values from case 1 but with a lateral dispersion added.

---

*See Notes (page 45)*
Case 4 a describes migration from an infinite slab source of 
10 m²/m in a parallel velocity field of 1 m/yr. The migration 
length is 500 meters (see figure 2.3).

To limit the amount of calculations to be done only the retention factor set R₂ is used. The rest of the parameters used are:

- Nuclide inventory: I₁ and I₂
- Leach duration: T₂ (10⁵ yrs)
- Boundary condition at x = 0: B₁ and/or B₂
- Peclet number for axial dispersion: P₂ (10)
- Lateral dispersion length: a_T = 5 m

Case 4 b

This case is an extension of case 4 a to a nonparallel velocity field which is described below. The rest of the parameters are taken directly from case 4 a.

The flow field can be visualized as that between two wells, one with an outflow of q m³/m/year the other with an equally large inflow, drilled through a permeable layer of unit thickness (see figure 2.4).

This generates a field with a potential ϕ which can be described as

\[ ϕ = \frac{q}{4 \pi} \ln \left( \frac{(x - x₁)^2 + y^2}{(x + x₁)^2 + y^2} \right) \]
Figure 2.4. Streamlines of the flow field in case 4 b.

The velocities in x- and y-direction (u and w respectively) can be derived by differentiation with respect to x and y which gives the velocity components as:

\[
u = -\frac{1}{\varepsilon} \frac{\partial \phi}{\partial x}
\]

\[
u = -\frac{q}{2 \pi \varepsilon} \left( \frac{x - x_1}{(x-x_1)^2 + y^2} - \frac{x + x_1}{(x+x_1)^2 + y^2} \right)
\]

\[
\omega = -\frac{1}{\varepsilon} \frac{\partial \phi}{\partial y}
\]

\[
\omega = -\frac{q \cdot y}{2 \pi \varepsilon} \left( \frac{1}{(x-x_1)^2 + y^2} - \frac{1}{(x+x_1)^2 + y^2} \right)
\]

The case describes the transport of dissolved radioactive material from a source situated at 10 m from the inflow well with dimensions and orientation as in figure 2.5 to a target line at x = 0. The total flow of radionuclides and concentration profile along the target line is studied.
To be able to compare the results from this case with results from the other cases we fix \( x_1 \) to 510 m and postulate a groundwater travel time = 500 years along the shortest streamline (the x-axis). This leaves us with a \( q = 346.6 \cdot \pi \cdot \varepsilon \cdot m^3/m \cdot \text{year} \) and:

\[
    u = 173.3 \left( \frac{x + 510}{(x+510)^2 + y^2} - \frac{x - 510}{(x-510)^2 + y^2} \right),
\]

\[
    w = 173.3 \frac{y}{(x-510)^2 + y^2} - \frac{1}{(x+510)^2 + y^2})
\]

**Case 5**

This case considers a medium of a set of parallel fractures and diffusion into the rock matrix separating them (see figure 2.6). The case has the same flowrate as cases 1-3. In other respects

**Figure 2.5.** Source arrangement in case 4 b.

**Figure 2.6.** Fracture arrangement in case 5
it describes a totally different physical situation. The parameters have been chosen so that the codes will be put to test by not giving only trivial results.

Nuclide inventory: \( I_2 \)
Leach duration: \( T_2 \) (10\(^5\) yrs)
Boundary condition: \( B_1 \) and/or \( B_2 \)
Migration length: \( L_1 \) (500 m)
Ground water velocity in the cracks: 500 m/yr
Peclet number in the cracks: \( P_2 \) (10)
Crack spacing: \( s = 5 \) m
Crack width: \( 2b = 10^{-4} \) m
Diffusivity in the rock matrix\(^1\): \( D_e = 10^{-12} \) m\(^2\)/s
Porosity of the rock matrix: \( \epsilon_p = 5 \cdot 10^{-3} \)
Bulk density of the rock matrix: \( \rho_p = 2700 \) kg/m\(^3\)

Volume based distribution coefficients in the matrix:

<table>
<thead>
<tr>
<th>Element</th>
<th>( K_v = \rho_p K_d )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cm</td>
<td>570</td>
</tr>
<tr>
<td>Np</td>
<td>80</td>
</tr>
<tr>
<td>U</td>
<td>30</td>
</tr>
<tr>
<td>Th</td>
<td>2300</td>
</tr>
<tr>
<td>Ra</td>
<td>1100</td>
</tr>
</tbody>
</table>

Case 6 a

This case is based on the set of parameters used in case 4 a but with the diffusion into the rock matrix added. For the matrix diffusion the rock blocks are assumed to be spheres of radius 2.5 m. The amount of solid material should be adjusted to correspond to case 5 i.e. a crack width of 10\(^{-4}\) m and a crack spacing of 5 m (crack porosity 2 \( \cdot \) 10\(^{-5}\)). The geometric description (source dimensions and migration length) is equivalent to that of case 4 a. The other parameter values used are:

Nuclide inventory: \( I_2 \)
Leach duration: \( T_2 \) (10\(^5\) yrs)
Boundary condition: \( B_1 \) and/or \( B_2 \)
Ground water velocity in the cracks: 500 m/yr

\(^1\) See Notes (page 45)
Peclet number in the cracks: $P_2 (10)$
Lateral dispersion length: $a_T = 5 \text{ m}$
Diffusivity in the rock matrix$^1$: $D_e = 10^{-12} \text{ m}^2/\text{s}$
Porosity of the rock matrix: $\varepsilon_p = 5 \cdot 10^{-3}$

Volume based distribution coefficients in the matrix:

<table>
<thead>
<tr>
<th>Element</th>
<th>$K_v = \rho_p K_d$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cm</td>
<td>570</td>
</tr>
<tr>
<td>Np</td>
<td>80</td>
</tr>
<tr>
<td>U</td>
<td>30</td>
</tr>
<tr>
<td>Th</td>
<td>2 300</td>
</tr>
<tr>
<td>Ra</td>
<td>1 100</td>
</tr>
</tbody>
</table>

Case 6 b

This case is an extension of case 6 a to a non-uniform velocity field. The velocity field used is described under case 4 b. The flowrate is, however, increased by a factor of 500. The rest of the parameters are taken from case 6 a.

Case 7

This case is based on the basic set of parameter values from case 1 with the addition of a mass transfer resistance between the liquid and the solid phase (see figure 2.7). The mass transfer rate is assumed to be described by a mass transfer coefficient.

A material balance on a unit volume of porous rock with an effective interface area rock/water = A m$^2$ can be written as:

$$\frac{\partial C_k}{\partial t} = \frac{\varepsilon}{\partial x} \frac{\partial^2 C_k}{\partial x^2} + \varepsilon (-\lambda_k C_k + \lambda_{k-1} C_{k-1}) - k_m A \left( C_k - \frac{N_k}{K_d} \right)$$

$$\frac{(1-\varepsilon) \rho_g \partial M_k}{\partial t} = (1-\varepsilon) \rho_g (-\lambda_k M_k + \lambda_{k-1} M_{k-1}) + k_m A \left( C_k - \frac{N_k}{K_d} \right)$$

$^1$ See Notes (page 45)
Figure 2.7. Illustration of the mass transfer resistance in case 7. The figure shows qualitatively the concentration distribution across a fracture.

The distribution coefficient, $K_d$, can be back-calculated from the retardation factors given in case 1 according to the following relation:

$$K_d = \frac{(R-1)\varepsilon}{(1-\varepsilon)\rho_s}$$

The following values should be assumed:

- $\varepsilon = 10^{-2} \text{ (m}^3/\text{m}^3\text{)}$
- $\rho_s = 2700 \text{ (kg/m}^3\text{)}$
- $k_{mA} = 0.10^{-5}, 10^{-4} \text{ and } 10^{-2} \text{ (year}^{-1}\text{)}$
3 RESULTS FROM LEVEL 1

3.1 INTRODUCTION

3.1.1 General

The compilation of the results presented in this report was made by the project secretariat based on data submitted to the secretariat by the project teams. For most of the calculated cases the following information was requested:

- The nuclide concentrations at the end of the migration path (activity units per cubic meter) as a function of time.

- Maximum concentrations, the times for the maxima and the times when the concentration is half of the maximum concentration.

- Execution time (CPU-seconds) and the time for one single precision floating point multiplication at the used computer installation.

For the two dimensional cases (cases 4 and 6) the nuclide flux (activity units per year) across an observation line was requested as a function of time together with the concentration distribution along the observation line at the time for maximum nuclide flux.

Most of the data were submitted to the project secretariat on magnetic tape but a few of the project teams sent only tabulated data. All data sent to the secretariat are available on microfiche(g) and on magnetic tape(k). Many project teams have also prepared more complete reports on their own work. A list of these reports can be found in Chapter 8. They are available on request from the authors.

3.1.2 Result presentation format

The data have been processed by the secretariat in order to facilitate the comparison of results from different codes. In Appendix 3 most of the results are presented. However, for case 1 only the results corresponding to the "Basic set" of parameter values are shown. The results for the other parameter values are discussed in section 3.3. The presentation in Appendix 3 comprises for each case the following items:

- Tables of maximum outlet concentration, time for the maximum and times for 10% of the maximum on both sides of the peak. Note that the 10% is used instead of the 50% requested from the project teams. The change was made to increase the sensitivity of the comparison.

j) and k) See Notes (page 46)
- Tables indicating the computational efforts. These tables contain the total time span (yrs) covered by the calculation, the equivalent number of arithmetic operations, defined as the CPU-time divided by the time for one floating point multiplication, and the number of arithmetic operations per year defined as the quotient between the values in the second and first columns. It should be noted that codes with automatic time stepping procedures can give considerably different values for the number of operations per year depending on the simulated time period. Furthermore there was no precision criterion stated in the case definitions. The data on CPU-usage are therefore no absolute measure on code efficiencies.

- Plots of the outlet concentration as a function of time. The curves are marked by numbers that are explained in the above mentioned tables of maximum concentrations.

For cases 4 and 6 the nuclide flux across the observation line has been recorded instead of concentrations and the presentation is complemented by the concentration distribution at the time of maximum flux.

The tabulated values in Appendix 3 have been calculated from the concentration (flux) versus time tables that were submitted to the secretariat and might therefore deviate slightly from the values originally submitted by the project teams. The maximum concentration and the time of the maximum were calculated from a cubic spline interpolation using five data points around the highest reported value. The times for 10% of the maximum concentration was calculated using linear interpolation. The uncertainties introduced in this way are deemed to be of minor importance compared to other uncertainties in the calculations. Concentrations less than 1E-15 activity units/m³ are not reported.

In section 3.2 a discussion on possible causes of differences in the results obtained by the various codes is presented. As the boundary conditions were not very strictly defined this discussion is focused on the influence of the various boundary conditions and their implementations. Section 3.3 gives the main conclusions that can be drawn from the cases at level 1. Finally in section 3.4 the sensitivity of the code intercomparison for various parameter values is discussed.

---

3.2 REASONS FOR DEVIATING RESULTS

One of the main goals of INTRACOIN level 1 is code verification. This implies a comparison of calculational results of the different codes and an understanding of deviations. In general, there are two sources of deviating results. First there might be computational errors. These can be broken up into:
a) Data input errors. Though the project teams had the opportunity to resubmit new results after a first intercomparison it is suspected that there are still errors of this type.

b) Programming errors. These might show up only for very specific parameter sets. A judgement is impossible without detailed knowledge of the code.

c) Inadequate numerical approximations. This could induce round-off errors and numerical instabilities for specific parameter sets.

d) Truncation errors. These could be the results of inadequate choice of discretization in space and time and also induce instabilities of the solution.

A second cause of deviating results is the use of different boundary conditions. First, the project teams were free to use their own choice of boundary conditions and second the definition of one of the boundary conditions in the benchmark cases is not unique (B2). Since the effect of varying boundary conditions is qualitatively well understood this gives a further means of code verification and, as a positive byproduct, information on the quantitative effect of the choice of boundary conditions is gained.

Before discussing the effects of boundary conditions (b.c.) and their implementation in numerical solution it is appropriate to give the mathematical formulation of various b.c. The correct choice of b.c. depends on the physical problem at hand and has been extensively discussed in the literature (Ref. 3). The choice of b.c. by the project teams was influenced by such considerations or dictated by the requirements of the models used.

A general formulation of a b.c. is given by

\[ \alpha C(x,y,z,t) + \beta \hat{n} \cdot \nabla C(x,y,z,t) = \gamma \]  

(3.1)

where \((x,y,z)\) are on the boundary \(\Gamma\), \(\hat{n}\) is a unit vector normal to the surface \(\Gamma\) and \(\alpha, \beta, \gamma\) are arbitrary functions of time on \(\Gamma\). Special choices of \(\alpha, \beta, \gamma\) correspond to realisations of the special physical problems. In order to be specific we consider the one-dimensional transport problem (cases 1 to 3), recognizing that extensions to higher space dimensions are trivial. The source is situated at \(x = 0\) m and the observation point at \(L = 500\) m \((L_1)\) or \(L = 5\,000\) m \((L_2)\), respectively.

At any point \(x\) the radionuclide flux is defined by

\[ j(x,t) = \epsilon \left( v C(x,t) - D \frac{\partial C(x,t)}{\partial x} \right) \]  

(3.2)
Downstream three b.c. have been considered:

a) A semi-infinite medium with

\[ \lim_{x_d \to \infty} C(x_d, t) = 0. \tag{3.3} \]

This b.c. is designated \( E_1 \). This is the standard b.c. for analytically solvable models. Numerical models have to specify a finite number for \( x_d \). Choosing a too small \( x_d \) yields too low maximum concentrations since flux is withdrawn at \( x_d \). The effect is, of course strongly dependent on the magnitude of retention.

b) Flow into a reservoir with infinite dilution, i.e.

\[ C(L, t) = 0 \tag{3.4} \]

This b.c. is designated \( E_2 \). The maximum concentrations must be lower than for \( E_1 \) since the concentration gradient at \( x=L \) is higher. It is, however, not clear that the implementations of \( E_2 \) used in this study has this effect. (See Note a), page 45).

c) A boundary impervious to dispersion, i.e.

\[ \frac{\partial C(x, t)}{\partial x} \bigg|_{x=L} = 0 \tag{3.5} \]

This b.c. is designated \( E_3 \). The maximum concentration must be higher and earlier than for \( E_1 \) since less flux crosses the observation point during the rising part of the chromatographic curve.

Also upstream several b.c. have been considered.

a) A concentration boundary, i.e.

\[ C(x=0, t) = \frac{I(t)}{\epsilon \nu \pi} u(T-t), \quad t>0. \tag{3.6} \]

where \( u(t) \) is the unit step function (ref. 4). This b.c. is designated \( B_1 \). It is the standard b.c. for analytically solvable models.

b) Fixing the influx by the source strength, i.e.

\[ j(x=0, t) = \frac{I(t)}{\pi T} u(T-t), \quad t>0. \tag{3.7} \]

where: \[ j = -\frac{\partial C}{\partial x} + \nu \epsilon \cdot C \]
We call this a flux boundary and denote it $B_2(F)$. Maximum concentrations must be lower and come later compared to $B_1$ since the concentration at $x=0$ has to be built up with time.

c) Fixing the flux discontinuity at $x=0$ by the source strength, i.e.

$$\lim_{\Delta \to 0} \left \{ j(A,t) - j(-A,t) \right \} = \frac{I(t)}{\epsilon FT} u(T-t), t>0. \quad (3.8)$$

We call this a source boundary and denote it $B_2(S)$. The reason is that this b.c. is equivalent to an extension of the integration domain to $x=\infty$, adding a source term

$$\frac{I(t)}{\epsilon FT} \delta(x) u(T-t), t>0. \quad (3.9)$$

to the conventional transport equation

$$\lim_{x \to -\infty} C(x_u,t) = 0 \quad (3.10)$$

as the new boundary condition. Also for this case analytical solutions are available. Maximum concentrations must be lower and come later compared to $B_2(F)$ since the region $x<0$ is available for contamination.

Table 3.1 shows which variants of b.c. were used by project teams for case 1, basic parameter set, and table 3.2 those for case 2 calculations.

From the general discussion on b.c. one expects for the first nuclide the following relationship for case 1

$$C_{\text{max}}(B_1) > C_{\text{max}}(B_2F) > C_{\text{max}}(B_2S) \quad (3.11a)$$

and

$$T_{\text{max}}(B_1) < T_{\text{max}}(B_2F) < T_{\text{max}}(B_2S) \quad (3.11b)$$

for fixed downstream b.c. and also

$$C_{\text{max}}(E_3) > C_{\text{max}}(E_1) \quad (3.12a)$$

and

$$T_{\text{max}}(E_3) < T_{\text{max}}(E_1) \quad (3.12b)$$

for fixed upstream b.c.

1) See Notes (page 46)
Table 3.1 Choice and implementation of boundary conditions for case 1, basic parameter set.

<table>
<thead>
<tr>
<th>Code</th>
<th>Upstream Boundary</th>
<th>Downstream Boundary</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 GETOUT VTT</td>
<td>B₁</td>
<td>E₁ (x_d = -)</td>
</tr>
<tr>
<td>2 GETOUT OMNI</td>
<td>B₁</td>
<td>E₁ (x_d = -)</td>
</tr>
<tr>
<td>3 UCB-NE</td>
<td>B₁ B₂(S)</td>
<td>E₁ (x_d = -)</td>
</tr>
<tr>
<td>4 RANCH</td>
<td>B₁ B₂(S)</td>
<td>E₁ (x_d = -)</td>
</tr>
<tr>
<td>5 RANCHN</td>
<td>B₁</td>
<td>E₁ (x_d = 900 m)</td>
</tr>
<tr>
<td>6 GEOS</td>
<td>B₂(F)</td>
<td>E₁ (x_d = 625 m)</td>
</tr>
<tr>
<td>7 SWENT</td>
<td>B₂(F)</td>
<td>E₁ (x_d = 3.750 m) E₃</td>
</tr>
<tr>
<td>8 SWIFT</td>
<td>B₂(F)</td>
<td>E₁ (x_d = 800 m)</td>
</tr>
<tr>
<td>9 TROUGH</td>
<td>B₁</td>
<td>E₁ (x_d = 2500 m)</td>
</tr>
<tr>
<td>10 TRUNN</td>
<td>B₁</td>
<td>E₁ (x_d = 3075 m)</td>
</tr>
<tr>
<td>11 METIS</td>
<td>B₁ B₂(F)</td>
<td>E₁ (x_d = 1700 m)</td>
</tr>
<tr>
<td>12 TRANSAT</td>
<td>B₁ B₂(F)</td>
<td>E₁ (x_d = 3250 m) E₃</td>
</tr>
<tr>
<td>13 DRAMA</td>
<td>B₂(F)</td>
<td>E₂*)</td>
</tr>
<tr>
<td>14 HTIDPWH</td>
<td>B₁ B₂(F)</td>
<td>E₃*)</td>
</tr>
<tr>
<td>15 MTIVTT</td>
<td>B₁</td>
<td>E₂*)</td>
</tr>
<tr>
<td>16 COLUMN</td>
<td>B₁</td>
<td>E₃</td>
</tr>
<tr>
<td>17 DPCT</td>
<td>B₂(S)</td>
<td>E₁ (x_d = 1000 m)</td>
</tr>
<tr>
<td>18 NUTRAN</td>
<td>B₂(S)</td>
<td>E₁ (x_d = -)</td>
</tr>
<tr>
<td>19 NWFT/DVM</td>
<td>B₂(F)</td>
<td>E₁ (x_d = -)</td>
</tr>
<tr>
<td>20 SWIFT II</td>
<td>B₂(F)</td>
<td>E₁ (x_d = 1430)</td>
</tr>
<tr>
<td>21 PORFLO</td>
<td>B₁</td>
<td>E₃</td>
</tr>
</tbody>
</table>

*) Comments to the downstream boundary condition used with DRAMA and the two HMT-versions are given in note a), page 45.

Table 3.2 Choice and implementation of boundary conditions for case 2.

<table>
<thead>
<tr>
<th>Code</th>
<th>Upstream Boundary</th>
<th>Downstream Boundary</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 RANCH</td>
<td>B₁</td>
<td>E₁ (x_d = -)</td>
</tr>
<tr>
<td>5 RANCHN</td>
<td>B₁</td>
<td>E₁ (x_d = 800 m)</td>
</tr>
<tr>
<td>6 GEOS</td>
<td>B₂(F)</td>
<td>E₁ (x_d = 625 m)</td>
</tr>
<tr>
<td>7 SWENT</td>
<td>B₂(F)</td>
<td>E₃</td>
</tr>
<tr>
<td>8 SWIFT</td>
<td>B₂(F)</td>
<td>E₁ (x_d = 800 m)</td>
</tr>
<tr>
<td>9 TROUGH</td>
<td>B₁</td>
<td>E₁ (x_d = 2500 m)</td>
</tr>
<tr>
<td>10 TRUNN</td>
<td>B₁</td>
<td>E₁ (x_d = 3050 m)</td>
</tr>
<tr>
<td>11 METIS</td>
<td>B₁ B₂(F)</td>
<td>E₁ (x_d = 1700 m)</td>
</tr>
<tr>
<td>12 TRANSAT</td>
<td>B₁</td>
<td>E₃</td>
</tr>
<tr>
<td>13 DRAMA</td>
<td>B₂(F)</td>
<td>E₂*)</td>
</tr>
<tr>
<td>14 HTIDPWH</td>
<td>B₁ B₂(F)</td>
<td>E₃*)</td>
</tr>
<tr>
<td>15 MTIVTT</td>
<td>B₁</td>
<td>E₂*)</td>
</tr>
<tr>
<td>16 COLUMN</td>
<td>B₁</td>
<td>E₃</td>
</tr>
<tr>
<td>17 DPCT</td>
<td>B₂(S)</td>
<td>E₁ (x_d = 1000 m)</td>
</tr>
<tr>
<td>18 NUTRAN</td>
<td>B₂(S)</td>
<td>E₁ (x_d = -)</td>
</tr>
<tr>
<td>19 NWFT/DVM</td>
<td>B₂(F)</td>
<td>E₁ (x_d = -)</td>
</tr>
<tr>
<td>20 SWIFT II</td>
<td>B₂(F)</td>
<td>E₁ (x_d = 1430)</td>
</tr>
<tr>
<td>21 PORFLO</td>
<td>B₁</td>
<td>E₃</td>
</tr>
</tbody>
</table>
The bulk of calculations has been made for $E_1 B_1$. Since requirements of accuracy and modelling were not precisely defined for benchmarking and numerical implementation of b.c. is not always exactly known a comparison of results on the percent level for $T_{\text{max}}$ and $C_{\text{max}}$ is impossible. In addition $C_{\text{max}}$ and $T_{\text{max}}$ have been interpolated from results submitted by project teams. Here another uncertainty is introduced. Hence, the values might not exactly coincide with those of the original maxima tables.

For the layered medium (case 2) in addition flux conservation and concentration continuity have to be imposed at interlayer boundaries:

$$\lim_{\delta \to 0} C(x_N - \Delta, t) = C(x_N + \Delta, t) \quad (3.13)$$

and

$$\lim_{\delta \to 0} j(x_N - \Delta, t) = j(x_N + \Delta, t) \quad (3.14)$$

where $x_N$ is the coordinate of the interlayer boundary.

Possible discrepancies in calculational results might be induced by

a) Approximations of these boundary conditions.

b) Smearing of the parameter discontinuities over the discretization lengths.

3.3 RESULTS FROM THE CODE INTERCOMPARISON

3.3.1 Case 1

As mentioned in Chapter 2 a number of parameter variations were defined for case 1. In table 3.3 a summary of the parameter variations calculated with the various codes is presented. As can be seen most of the codes have calculated the basic set whereas the number of codes that have been applied to the other parameter variations varies strongly. The code GARD2S does not treat dispersion and has thus only been applied to cases with the $P_1$ variant of the Peclet number.

The discussion below is carried through only for the basic set. The other parameter variations are discussed in section 3.4 and the results are available on microfiche.
Tab 3.3 Case 1, parameter combinations calculated with various codes

<table>
<thead>
<tr>
<th></th>
<th>1 R1</th>
<th>1 R2</th>
<th>1 R1</th>
<th>1 R2</th>
</tr>
</thead>
<tbody>
<tr>
<td>GETOUTO</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>GETOUTV</td>
<td>XXX</td>
<td>XXX</td>
<td>XXX</td>
<td>XXX</td>
</tr>
<tr>
<td>GARD 25</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>UCB-NE</td>
<td>XXX</td>
<td>XXX</td>
<td>XXX</td>
<td>XXX</td>
</tr>
<tr>
<td>RANCH</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>RANCHN</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>GEOS</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>SWENT</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>SWIFT</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>SWIFT II</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>TROUGH</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>TRUCHN</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>TRANSAT</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>DPC1</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>METIS</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>MTRAM</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>COLUMN</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>MWT/DVM</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>MT1DPM</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>MT1UT</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>ORJAM</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>PORFLO</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
</tbody>
</table>
The results for the basic set of case 1 are presented on pages 2-17 in Appendix 3 and in figures 3.1 - 3.15. Figure 3.1 shows the maximum concentration for the \( I_1R_1 \)-run with the different codes. Results produced using the same boundary conditions are connected with lines and distinguished by the use of different markers. The figures 3.2 - 3.4 show the time for 10% of the maximum concentration on the rising part of the chromatographic curve \( T_1(10\%) \), the time of the maximum concentration \( T(C_{\text{max}}) \) and the time for 10% of the maximum concentration on the sinking part of the curve, \( T_1(10\%) \). This sequence of figures is then repeated for the other basic set runs, i.e. figures 3.5 - 3.8 for \( I_1R_2 \), 3.9 - 3.11 for \( I_2R_1 \) and 3.12 - 3.15 for \( I_2R_2 \).

Simple analytical solutions are readily available for the first nuclide with the boundary conditions \( E_1B_1 \) and \( E_1B_2(S) \) (e.g. Ref. 3). Such a solution is used below for \( E_1B_1 \) as an exact solution to compare the different codes against.

**Calculations with \( E_1B_1 \)**

This is the most commonly used boundary condition. It was calculated with the codes GETOUTV, GETOUTO, UCB, RANCH, RANCHN, TRUCHN, METIS and TRANSAT (first nuclide only). The exact solution for the first nuclide with this boundary condition is given in table 3.4. A comparison with exact results for \( C_{\text{max}} \) is shown in table 3.5. The agreement is reasonably good. All deviations are less than 5%.

<table>
<thead>
<tr>
<th>Basic parameter set</th>
<th>Nuclide</th>
<th>( C_{\text{max}} ) [act./m(^3)]</th>
<th>( T_{\text{max}} ) [yr]</th>
</tr>
</thead>
<tbody>
<tr>
<td>( I_1R_1 )</td>
<td>( ^{234}\text{U} )</td>
<td>3.935E-6</td>
<td>1.64E+5</td>
</tr>
<tr>
<td>( I_1R_2 )</td>
<td>( ^{234}\text{U} )</td>
<td>8.151E-6</td>
<td>6.20E+4</td>
</tr>
<tr>
<td>( I_2R_1 )</td>
<td>( ^{245}\text{Cm} )</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>( I_2R_2 )</td>
<td>( ^{245}\text{Cm} )</td>
<td>3.829E-7</td>
<td>2.55E+4</td>
</tr>
</tbody>
</table>

For the daughter nuclides and case 1 a larger scatter is recognized in \( C_{\text{max}} \) and \( T_{\text{max}} \) values. However, in general a rough agreement is seen whereas time distributions from GETOUT very often show a peculiar shape (see e.g. curve 1 page 13 in Appendix 3).
In the analytical solutions in GETOUT negative square-root arguments can occur for the daughter nuclides. The deviating GETOUTO results for the second and third member (Th-230 and Ra-226) probably occur because dispersion is not included for the daughter nuclides in this GETOUT-version. In GETOUTV instead, terms that can not be calculated by using elementary transcendental functions are skipped and a warning is issued in the printout. Both these strategies seem sometimes to yield unreliable results.

Going more into detail one recognizes that in general METIS results for $C_{\text{max}}$ are too high and $T_{\text{max}}$ too large. The reason is that upstream diffusion from the source was allowed. This means that the source strength is higher in the METIS runs than in the runs with the other codes. TRUCHN results give too early an increase of concentration, which probably is a result of approximating porous medium transport with instationary diffusion in a thin rock slice.

Calculated with $E_2B_1$

This boundary condition combination was run only with MMTVTT. Therefore no real comparison can be made. However, the results sometimes seem to deviate more than can be explained from differences in boundary condition implementations.

Calculated with $E_3B_1$

Three codes, PORFLO, COLUMN and MMTIDPNL implemented this boundary condition. In addition there are TRANSAT calculations for the first nuclide for $I_1R_1$.

For the first nuclide of case 1 the relations (3.11) and (3.12) are fulfilled. The COLUMN and PORFLO $C_{\text{max}}$ results are always
higher and, mostly, earlier than those of MKT. This might be an effect of different boundary condition implementation (see note a, page 45). For the daughter nuclides no consistent picture is seen.

**Calculations with E₁B₂(S)**

Only UCB-NE, RANCH (I₁R₁ only) DPCT and NUTRAN have calculated case 1 benchmarks with this boundary condition. The conditions (3.11) and (3.12) are well fulfilled. As is to be expected deviations from B₁R₁ are less for the small retention factors. Good agreement is seen for the parameter set where both codes have performed calculations. However, there are some results that should be commented. NUTRAN does not treat daughter nuclides in a rigorous way. This is the probable reason for some significantly deviating results (see I₂R₁ and I₂R₂). In the I₂R₂ run the results for the first nuclide also deviate significantly more than can be explained by e.g. boundary condition implementation.

**Calculations with E₁B₂(F)**

Calculations were performed with GEOS, SWENT (case 1 I₁R₁), SWIFT, METIS, TRANSAT (first nuclide for I₁R₁), SWIFT II and NWFT/DVM. Most of the results nicely fulfill the relations (3.11) and (3.12). The results in general also agree reasonably well with each other. The maximum concentrations from NWFT/DVM for the daughter nuclides in the I₁R₁-run are, however, too high. In the other runs there is a slight tendency towards high maximum concentrations for the second nuclide. Also the maximum concentrations predicted by GEOS are up to 10% lower than those predicted by the other codes. This is a consequence of too short a system length (650 m), the shortening being especially apparent for the low retention factor set R₂.

**Calculations with E₂B₂**

A single code only, DRAMA has implemented this boundary condition. Due to the solution approach the results have oscillating structure which has not been sufficiently smoothed. The oscillations are relatively large (e.g. for I₂R₁) and, hence, the C_{max} - T_{max} - tables do not give a representative picture. A comparison with results from other codes is therefore not performed.

**Calculations with E₂B₂(F)**

Results are available from SWENT and MNDTDPNL calculations. For C_{max} and T_{max} they differ strongly in most cases. In general the results of SWENT agree with the bulk of E₁B₁ results, except for
the third nuclide of case 1, $I_1 R_2$, where the selected time step scarcely fulfills the requirements stated in the code characterization (see Appendix 2). For the first nuclide the effect of decreasing $C_{\text{max}}$ for boundary condition $B_2$ in comparison with $B_1$ is compensated by boundary condition $E_3$ in comparison with $E_1$. Also for daughter nuclides such a compensation is expected and seen for the SWENT results. A characteristic of the MMT1DPNL results is the early rise of the concentration versus time distribu-

3.3.2 Case 2

The results for case 2 can be found in Appendix 3 (pages 18-33) and in figures 3.16 - 3.30. In the figures the $C_{\text{max}}$, $T_{\text{max}}$, $T+(10\%)$ and $T-(10\%)$ values have been plotted for the various codes. The different boundary conditions are distinguished by using different markers.

The general tendency for case 2 is that the agreement between the codes is better than in case 1. The reason for this is partly that the dispersivity is smaller and partly that a major portion of the transport time comes from the first zone, i.e. the first 50 m of the migration path. The comparison is thus less sensitive in case 2 than in case 1. Some deviations occur and may be explained either by oscillating and/or poorly convergent solutions in the discrete parcel-random walk algorithm codes or by a different interpretation of the dispersion coefficient from the given Peclet number. Most of the participants have used the individual zone lengths as the characteristic length in the Peclet number definition leading to different dispersion coefficients in different zones. Due to an unfortunate definition of the Peclet number in the notation list some of the codes have been run using the total migration path length as characteristic length. This probably accounts for some of the deviations obtained with DRAMA, TRUCHN, COLUMN, NWFT/DVM and NUTRAN. The four individual runs are discussed below.

$I_1 R_1$ (pages 18-21 in Appendix 3):

The random walk algorithm codes seem to have had problems to deliver reliable results. TRUCHN and COLUMN give low concentrations probably because of the above mentioned interpretation of the dispersivity. Furthermore NUTRAN and NWFT/DVM give results that deviate more than can be explained by either different boundary condition implementations or different interpretations of the dispersivity.

$I_1 R_2$ (pages 22-25 in Appendix 3):

The agreement between the codes is extremely good with the excep-

...
rently deviating \( C_{\text{max}} \) for DPCT (see figure 3.20) is due to small oscillations and therefore of little significance to the quality of the solution. As can be seen in Appendix 3 the chromatographic peaks from NUTRAN do not coincide with those from the bulk of the codes. For the first nuclide the peak comes late, whereas the tail is too short for the daughter nuclides. The maximum concentrations from NWFT/DVM are too low, especially for third chain member.

\( I_2 R_1 \) (pages 26-29 in Appendix 3):

The first nuclide (Cm-245) has decayed in this run. The agreement between the codes is good for the other two nuclides with the exception for NWFT/DVM, DRAMA and COLUMN. The reason for these deviations is partly the different treatment of dispersion and partly different boundary condition implementations. Due to some oscillations in the DRAMA results they differ significantly from the COLUMN results for the first nuclide.

\( I_2 R_2 \) (pages 30-33 in Appendix 3):

Except for NWFT/DVM, DRAMA and COLUMN the results agree fairly well. For explanation of the deviating results, see above.

3.3.3 Case 3

The results from case 3, which are shown on pages 34-49, in Appendix 3, are more scattered than those from both case 1 and case 2. In case 3 it is more difficult to draw conclusions about the reasons for the deviations than in the previous cases because different discretizations of the continuously decreasing retardation factors might have affected the results. The only deviations that cannot be explained by differences in boundary conditions and discretizations are the results for the second nuclide from DRAMA in the \( I_1 R_1 \) run (see pages 34 and 36 in Appendix 4) and some of the results from NWFT/DVM. These results are probably due to a poorly convergent solutions. In the \( I_2 R_2 \)-run a peculiar effect in the form of a wave-pattern due to frequent mesh redistributions can be seen for COLUMN (page 47 in Appendix 4).

3.3.4 Case 4

In case 4, SWIFT, SWENT, SWIFT II, DPCT, NUTRAN and METIS have been run under comparable conditions. The only runs that were made with enough codes to give a meaningful comparison are those of case 4a and which therefore are the only runs discussed here (see also pages 50-65 in Appendix 3). The SWIFT results are presented only as concentration distribution along the observation line at the time of maximum flux and the NUTRAN results only
show the flux versus time. The rest of the results are shown both ways.

The results are in good agreement for the boundary condition combination $E_1 B_2$ taking into account that the flux reported from METIS was integrated only over half of the flow domain. However, the peak from NUTRAN comes early and is higher than the bulk of the results. The apparently high fluxes are due to an input error. All fluxes should be reduced with a factor 0.6.

The run with METIS for $E_1 B_1$ has yielded concentrations which are too high. This is a result of extending the modelled domain to negative $x$-coordinates in combination with a constant concentration at $x=0$. The amount of nuclides fed from the source is therefore larger in this run.

It should be noted that because the only analytical code available for handling the two-dimensional problem (UCB-NE) omits axial dispersion, no means exists to judge objectively whether a result is "true" or not.

Case 4 b was not run by a large enough number of codes to give a meaningful comparison and has therefore been left out of this discussion. However, the numerical results for the $I_1 R_2$- and $I_2 R_2$-runs are shown on pages 66-79 in Appendix 3.

3.3.5 Case 5

Only the run for inventory $I_2$ was run by a large enough number of codes to give a meaningful comparison (see pages 84-87 in Appendix 3. For completeness the results for the $I_1$-run are shown on pages 80-83 in the appendix).

Of the codes that have participated in case 5 NUCDIF and TRANSMIT only treat single nuclides. The results from these codes for the second nuclide (Np-237) have therefore been produced assuming that the first nuclide (Cm-245) decays completely to Np-237 in the source.

The TRUCHN result for the first nuclide is high. This is probably caused by numerical dispersion. It should be noted that the first nuclide in this case has decayed strongly and that the concentrations are consequently very low.

3.3.6 Case 6

Case 6 has not been tackled by a large enough number of project teams to give a meaningful code intercomparison and is therefore left out of this discussion. For completeness, however, the results for case 6 a ($I_2$) are shown on pages 88-94 in Appendix 3 and for case 6 b ($I_2$) on pages 95-101.
3.3.7 Case 7

Case 7 was run by the codes TROUGH, COLUMN, UCB-NE, GEOS and DRAMA. The results are presented on pages 102-117 in Appendix 3.

The results in terms of maximum concentrations seem to be slightly scattered for identical parameter values. This is probably mainly due to differences in discretizations and boundary conditions. The most interesting result is, however, the relative insensitivity of the maximum concentrations to variations of mass-transfer rate ($k_mA$-value). Although the shapes of the concentration versus time curves change drastically when $k_mA$ goes from zero to infinity (compare the figures in Appendix 3) the maximum concentrations only vary within one and a half orders of magnitude.

3.4 SENSITIVITY OF THE CODE INTERCOMPARISON TO PARAMETER VARIATIONS

The presentations in sections 3.2 and 3.3 have for case 1 been based only on the "Basic set" of parameter values, i.e. a Peclet number of 10, a leach duration of 100,000 years and a migration length of 500 m. The sensitivity of the comparison for other parameter values can be estimated with reference to the figures 3.31 - 3.34. Each of these figures consists of six pages out of which two deal with the variation of the Peclet number, two with leach duration and two with migration length. It should be noted that the x-axes do not correspond to any scale, but merely carry labeled values. This means that no interpolation between the plotted points is possible.

Studying the first pages of the figures 3.31 - 3.34 one sees immediately that the spread of results is larger by far at the low Peclet number (high dispersivity). Some of the codes have been taxed beyond what they were designed to cope with at Peclet number equals 1. This is especially the case for GETOUTV. As can be seen from the figures the Peclet number is the parameter that has the greatest impact on the sensitivity of the code intercomparison.
SUMMARY OF RESULTS AND RECOMMENDATIONS FOR FUTURE BENCHMARK STUDIES

The first level of INTRACOIN has addressed the question of verifying the solutions of the transport-equation performed with 22 codes based on a number of different algorithms. This has been done for seven different cases ranging from simple one-dimensional transport in a porous medium with constant parameters to a two-dimensional transport in a fractured medium with diffusion into the rock matrix.

The normal procedure for verifying a numerical algorithm is to compare the results with an analytical solution to the problem. In some of the INTRACOIN level 1 cases this has not been possible because the problem have not been analytically solved. Intercomparison of results from different numerical programs has therefore also been used.

The algorithms applied to these problems are both analytical solutions and numerical schemes including finite differences, finite elements, the method of characteristics, the spectral method and the discrete parcel random walk algorithm. Some of the algorithms are primarily designed to handle predominantly advective or predominantly dispersive problems and can thus not be expected to give unconditionally reliable results in all ranges of parameter values. The intention has been to give, via the choice of parameter values, a reasonably sensitive intercomparison with little or no attention payed to the realism of the data.

It has been shown in section 7.4 that the choice of Peclat number for the basic set in case 1 (Pe=10) has given a moderately sensitive intercomparison and that choosing a still lower value would have given a higher sensitivity in the comparison.

The results from INTRACOIN level 1 show that the agreement between the results from the participating codes in general is good. Most of the deviating results have been explained either by discrepancies in the implementation of boundary conditions, deviating interpretation of input data or as a result of truncation errors (coarse discretization in space or time domain).

Some of the codes that are based on the discrete parcel random walk algorithm or particle tracking seem to need some "finger tip feeling" from the user in order to yield reliable results, especially for high dispersion coefficients (low Peclet number) where the statistical simulation of the dispersion gives rise to a statistical noise that needs to be filtered with care.

The low Peclet number has also caused problems for the early analytical solutions in the participating GETOUT-versions (GETOUTV
and GETOUTO). For high dispersion coefficient there is a rather high likelihood for negative square-root arguments to occur in the expressions for the daughter nuclides when dispersion is included. As described in section 3.2.1 the two GETOUT-versions have solved this dilemma in different manners, neither giving unconditionally reliable results.

It is believed that the results presented in this report can serve as a good data base for future code testing. However, this does not exclude a need for further bench-mark studies in the future. In order to give unambiguous results future studies should involve fewer but more firmly designed cases. Thus should:

- the boundary conditions and their numerical implementations be stringently defined for all boundaries,
- the discretization of continuously varying properties be stringently defined and
- the parameter values be chosen to give an optimal sensitivity in the comparison.
- an accuracy requirement be defined.

If such carefully designed bench-mark studies are combined with convergence test studies (varying discretizations of the modelled domain) it is believed that they will contribute significantly to the "finger tip feeling" that is vital in the handling of numerical codes. Although majority vote comparisons seems to be a feasible approach to the bench-mark problem, the development of rigorous and well programmed analytical solutions is of utmost importance in the quality assurance process.
NOTES

a) The use of the E₂ boundary condition was stated only for the DRAMA and MMTVTT results. In these codes particles that leave the modelled domain by both convection and dispersion have no means for reentering. This means that the dispersive flux goes one way across the boundary and the nuclide concentrations are discontinous at the boundary. The boundary condition used with MMTIDPML is the same but was denoted E₃ by the project team.

b) Inventory (arbitrary units of activity) at time t is to be calculated according to Bateman's equations:

\[ \frac{dI_k}{dt} = \lambda_k (I_k - I_{k-1}) \]

c) Boundary conditions B₁ and B₂ were given either as alternatives or complements.

d) This will permit comparisons between models which do or do not include longitudinal dispersion.

e) The first set corresponds to a rock case, the second to a salt case. Here proposed retention factors have been slightly modified from the originally proposed ones to allow for a sensible contribution of repository inventory of short-lived daughters. Note the unusual low R for curium. All values are intended to represent oxidising conditions. This is not realistic but necessary to make the comparison sensible.

f) Water velocity has been kept constant since only the combination v/R enters the transport equation, and the Peclet number is varied independently.

g) A constant Peclet number means that the dispersivity increases from layer 1 to layer 3.

h) The idea behind this hypothetical analytical form is an assumed decrease of retention factors due to a gradual change in redox potential and/or porosity along the migration path.

i) To clarify the nomenclature concerning the diffusivity of the rock matrix the following formulas are given:

Diffusivity in the pores

\[ D_p = D_w \cdot \frac{\delta}{T^2} \]
Effective diffusivity

\[ D_e = D_p \cdot e_p \]

Apparent diffusivity

\[ D_a = \frac{D_e}{K_{p} + e_p} \]

j) Available from:

Studsvikbiblioteket
S-611 82 NYKÖPING
Sweden

k) Contact:

Swedish Nuclear Power Inspectorate
Box 27106
S-102 52 STOCKHOLM
Sweden

l) In the form

\[ \frac{\partial C}{\partial t} = - \frac{\partial j}{\partial x} - \lambda R C \]
### NOMENCLATURE

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
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<tbody>
<tr>
<td>A</td>
<td>interfacial area per unit volume</td>
</tr>
<tr>
<td>a</td>
<td>dispersion length</td>
</tr>
<tr>
<td>(a_T)</td>
<td>lateral dispersion length</td>
</tr>
<tr>
<td>B</td>
<td>boundary condition</td>
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<tr>
<td>2b</td>
<td>crack width</td>
</tr>
<tr>
<td>C</td>
<td>nuclide concentration</td>
</tr>
<tr>
<td>(C_k(x,t))</td>
<td>concentration of nuclide (k)</td>
</tr>
<tr>
<td>D</td>
<td>dispersion coefficient</td>
</tr>
<tr>
<td>(D_a)</td>
<td>apparent diffusivity</td>
</tr>
<tr>
<td>(D_e)</td>
<td>effective diffusivity</td>
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<tr>
<td>(D_p)</td>
<td>diffusivity in the pores</td>
</tr>
<tr>
<td>(D_w)</td>
<td>diffusivity in unconfined water</td>
</tr>
<tr>
<td>F</td>
<td>cross section for flow of contaminated water at inlet</td>
</tr>
<tr>
<td>(F_k(t))</td>
<td>injection rate at inlet for nuclide (k)</td>
</tr>
<tr>
<td>G and H</td>
<td>constants for retention factor variation in case 3</td>
</tr>
<tr>
<td>I</td>
<td>nuclide inventory at time zero</td>
</tr>
<tr>
<td>(I_k(t))</td>
<td>inventory of nuclide (k) at time (t)</td>
</tr>
<tr>
<td>(j(x,t))</td>
<td>nuclide flux</td>
</tr>
<tr>
<td>(K_d)</td>
<td>mass based distribution coefficient</td>
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<tr>
<td>(K_v)</td>
<td>volume based distribution coefficient</td>
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<tr>
<td>(k)</td>
<td>nuclide index</td>
</tr>
<tr>
<td>(k_m)</td>
<td>mass-transfer coefficient</td>
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<tr>
<td>(l)</td>
<td>migration length</td>
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<tr>
<td>(M_k)</td>
<td>concentration of nuclide (k) in solid rock</td>
</tr>
<tr>
<td>N</td>
<td>index for layer number</td>
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<tr>
<td>(P_e)</td>
<td>Peclet number (P_e = v \cdot l/D = l/a)</td>
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<tr>
<td>(q)</td>
<td>source strength for two-dimensional flow</td>
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<tr>
<td>R</td>
<td>retention factor</td>
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<tr>
<td>s</td>
<td>crack spacing</td>
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<tr>
<td>T</td>
<td>leaching duration</td>
</tr>
<tr>
<td>(t)</td>
<td>time ((t = 0) at start of leaching)</td>
</tr>
<tr>
<td>(t_{1/2})</td>
<td>half-life</td>
</tr>
<tr>
<td>(u)</td>
<td>(x) - component of water velocity (2-D cases)</td>
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<tr>
<td>(u(t))</td>
<td>unit step function</td>
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v  water velocity
w  y-component of water velocity (2-D cases)
x  coordinate along migration path
x_d  x-coordinate of the downstream boundary of the modelled domain.
x_N  x-coordinate of the N:th interlayer boundary
x_u  x-coordinate of the upstream boundary of the modelled domain
y  coordinate perpendicular to migration path

Greek letters

δ  constrictivity
δ(x)  Dirac delta function
Δ  small offset in x
ε  effective porosity
ε_p  block porosity
λ_k  decay constant of nuclide k
ρ_p  bulk density of the rock matrix
ρ_g  density of the rock grains
τ²  tortuosity
φ  potential function for two-dimensional flow
REFERENCES


2 Nuclide half-lives are from Nuclear Data Sheets. The volumes used for different nuclides are:

\[
\begin{align*}
^{226}\text{Ra} & \quad \text{vol 20 p 119 (1977)} \\
^{230}\text{Th} & \quad \text{vol 20 p 139 (1977)} \\
^{233}\text{U} & \quad \text{vol 24 p 289 (1978)} \\
^{234}\text{U} & \quad \text{vol 21 p 493 (1977)} \\
^{237}\text{Np} & \quad \text{vol 23 p 71 (1978)} \\
^{245}\text{Cm} & \quad \text{vol 19 p 143 (1976)}
\end{align*}
\]


**LIST OF PROJECT TEAM REPORTS**

1. A. Bundi, J. Hadermann and F. Rösel, EIR Calculations for INTRACOIN Level 1 Benchmarks
   EIR internal report, TM-45-82-34 (12/7/82)
   and Corrigenda 21/9/82

2. C.R. Cole, Description of INTRACOIN benchmark cases as run with WMTID
   Pacific Northwest Laboratory, March 1982

3. P. Goblet, INTRACOIN Niveau 1, Etude de cas-types au moyen du code METIS
   Centre d’Informatique Géologique, LHM/RD/82/59

4. M. Gülker, E. Bülow and L. Heredia, INTRACOIN Level 1
   Benchmark Calculations with Code SWIFT
   Projekt Sicherheitsstudien Entsorgung, PSE-No. 82/48

5. J. Hadermann and F. Rösel, INTRACOIN Benchmark Calculations
   with Code RANCH: Level 1
   EIR internal report, TM-45-82-3 (1/2/82)

6. J. Hadermann and F. Rösel, INTRACOIN Level 1 Benchmark Calculations
   with EIR Codes CONZRA, RANCH and RANCHN
   EIR-Bericht No. 491 (March 1983), NAGRA, NTB-83-10 (March 1983)

7. R. Hopkirk, I. Schvannes
   TROUGH and INTRACOIN level 1. Polydynamics Research Report RR-6,
   Zürich, June 1982.

8. M. Magnusson, A. Rasmuson and I. Neretnieks, INTRACOIN,
   Results of codes TRUCHN and NUCDIF developed at Dept. of Chemical
   Engineering, Royal Institute of Technology, Stockholm,

9. F. Rösel and J. Hadermann, INTRACOIN Level 1 Calculations
   with Code RANCHN
   EIR internal report, TM-45-83-9 (7/2/83)

10. Application of the finite-difference code SWENT and the finite-element code FTRANS to benchmark radionuclide transport calculations
    INTERA Environmental Consultants, Inc., draft, April 1982

11. Calculations for the INTRACOIN project level 1 NRPB-report
Fig. 3.1 Maximum concentrations calculated with different codes for case 1 with the basic set of parameter values. Inventories and retardation factors are I1R1. Results with the same boundary conditions are connected with lines.
Fig. 3.2 Times for 10% of maximum concentration before (lower), after (upper) and time for maximum concentration (middle) computed with different codes for case 1 with basic set parameter values. The nuclides is U-234 with inventory and retention factor according to I1R1.
Fig. 3.3 Times for 10% of maximum concentration before (lower), after (upper) and time for maximum concentration (middle) computed with different codes for case 1 with basic set parameter values. The nuclide is Th-230 with inventory and retention factor according to I1R1.
Fig. 3.4 Times for 10% of maximum concentration before (lower), after (upper) and time for maximum concentration (middle) computed with different codes for case 1 with basic set parameter values. The nuclide is Ra-226 with inventory and retention factor according to I1R1.
Fig. 3.5  Maximum concentrations calculated with different codes for case 1 with the basic set of parameter values. Inventories and retardation factors are 1R2. Results with the same boundary conditions are connected with lines.
Fig. 3.6 Times for 10% of maximum concentration before (lower), after (upper) and time for maximum concentration (middle) computed with different codes for case 1 with basic set parameter values. The nuclide is U-234 with inventory and retention factor according to I1R2.
Fig. 3.7 Times for 10% of maximum concentration before (lower), after (upper) and time for maximum concentration (middle) computed with different codes for case 1 with basic set parameter values. The nuclide is Th-230 with inventory and retention factor according to I1R2.
Fig. 3.8 Times for 10% of maximum concentration before (lower), after (upper) and time for maximum concentration (middle) computed with different codes for case 1 with basic set parameter values. The nuclide is Ra-226 with inventory and retention factor according to I1R2.
Fig. 3.9 Maximum concentrations calculated with different codes for case 1 with the basic set of parameter values. Inventories and retardation factors are I2R1. Results with the same boundary conditions are connected with lines.
Fig. 3.10 Times for 10% of maximum concentration before (lower) and after (upper) and time for maximum concentration (middle) computed with different codes for case 1 with basic set parameter values. The nuclide is Np-237 with inventory and retention factor according to I2R.
Fig. 3.11 Times for 10% of maximum concentration before (lower), after (upper) and time for maximum concentration (middle) computed with different codes for case 1 with basic set parameter values. The nuclide is U-233 with inventory and retention factor according to I2R1.
Fig. 3.12 Maximum concentrations calculated with different codes for case 1 with the basic set of parameter values. Inventories and retardation factors are I2R2. Results with the same boundary conditions are connected with lines.
Fig. 3.13 Times for 10% of maximum concentration before (lower), after (upper) and time for maximum concentration (middle) computed with different codes for case 1 with basic set parameter values. The nuclide is Cm-245 with inventory and retention factor according to I2R2.
Fig. 3.14 Times for 10% of maximum concentration before (lower), after (upper) and time for maximum concentration (middle) computed with different codes for case 1 with basic set parameter values. The nuclide is Np-237 with inventory and retention factor according to I2R2.
Fig. 3.15 Times for 10% of maximum concentration before (lower), after (upper) and time for maximum concentration (middle) computed with different codes for case 1 with basic set parameter values. The nuclide is U-233 with inventory and retention factor according to I2R2.
Fig. 3.16 Maximum concentrations calculated with different codes for case 2 with the basic set of parameter values. Inventories and retardation factors are I1R1. Results with the same boundary conditions are connected with lines.
Fig. 3.17 Times for 10% of maximum concentration before (lower), after (upper) and time for maximum concentration (middle) computed with different codes for case 2 with basic set parameter values. The nuclide is U-234 with inventory and retention factor according to IIR1.
Fig. 3.18 Times for 10% of maximum concentration before (lower), after (upper) and time for maximum concentration (middle) computed with different codes for case 2 with basic set parameter values. The nuclide is Th-230 with inventory and retention factor according to IIIR1.
Fig. 3.19 Times for 10% of maximum concentration before (lower), after (upper) and time for maximum concentration (middle) computed with different codes for case 2 with basic set parameter values. The nuclide is Ra-226 with inventory and retention factor according to IIRl.
Fig. 3.20 Maximum concentration calculated with different codes for case 2 with the basic set of parameter values. Inventories and retardation factors are I1R1. Results with the same boundary conditions are connected with lines.
Fig. 3.21 Times for 10% of maximum concentration before (lower), after (upper) and time for maximum concentration (middle) computed with different codes for case 2 with basic set parameter values. The nuclide is U-234 with inventory and retention factor according to I1R2.
Fig. 3.22 Times for 10% of maximum concentration before (lower), after (upper) and time for maximum concentration (middle) computed with different codes for case 2 with basic set parameter values. The nuclide is Th-230 with inventory and retention factor according to I1R2.
Fig. 3.23 Times for 10% of maximum concentration before (lower), after (upper) and time for maximum concentration (middle) computed with different codes for case 2 with basic set parameter values. The nuclide is Ra-226 with inventory and retention factor according to I1R2.
Fig. 3.24 Maximum concentrations calculated with different codes for case 2 with the basic set of parameter values. Inventories and retardation factors are I2R1. Results with the same boundary conditions are connected with lines.
Fig. 3.25 Times for 10% of maximum concentration before (lower), after (upper) and time for maximum concentration (middle) computed with different codes for case 2 with basic set parameter values. The nuclide is Np-237 with inventory and retention factor according to I2R1.
Fig. 3.26 Times for 10\% of maximum concentration before (lower), after (upper) and time for maximum concentration (middle) computed with different codes for case 2 with basic set parameter values. The nuclide is U-233 with inventory and retention factor according to I2R1.
Fig. 3.27 Maximum concentrations calculated with different codes for case 2 with the basic set of parameter values. Inventories and retardation factors are 12R2. Results with the same boundary conditions are connected with lines.
Fig. 3.28 Times for 10% of maximum concentration before (lower), after (upper) and time for maximum concentration (middle) computed with different codes for case 2 with basic set parameter values. The nuclide is Cm-245 with inventory and retention factor according to I2R2.
Fig. 3.29 Times for 10% of maximum concentration before (lower), after (upper) and time for maximum concentration (middle) computed with different codes for case 2 with basic set parameter values. The nuclide is Np-237 with inventory and retention factor according to I2R2.
Fig. 3.30 Times for 10% of maximum concentration before (lower), after (upper) and time for maximum concentration (middle) computed with different codes for case 2 with basic set parameter values. The nuclide is U-233 with inventory and retention factor according to I2R2.
Fig 3.31-1.a Maximum concentration calculated with different values of the Peclet Number. Inventory and retention factors are I1R1. All runs were made with concentration boundary condition at source(B1). Note that interpolation between Peclet Number values is not possible.
Fig 3.31-1.b Same as fig. 3.31-1.a but with source boundary condition (B2).
Fig 3.31-2.a Maximum concentration calculated with different values for the Leach Duration. Inventory and retention factors are I1R1. All runs were made with concentration boundary condition at the source (B1). Note that interpolation between different Leach duration values is not possible.
Fig 3.31-2.b Same as fig. 3.31-2a but with source boundary condition (B2).
Fig 3.31-3.a Maximum concentration calculated with different Migration Length. Inventory and retention factors are 11R1. All runs were made with concentration boundary condition at the source(B1). Note that interpolation between different Migration Length is not possible.
Fig 3.31-3.b Same as fig. 3.31-3.a but with source boundary condition (B2).
Fig 3.32-1.a Maximum concentration calculated with different values of the Peclet Number. Inventory and retention factors are $10^2$. All runs were made with concentration boundary condition at source (B1). Note that interpolation between Peclet Number values is not possible.
Fig 3.32-1.b Same as fig. 3.32-1.a but with source boundary condition (B2).
Fig 3.32-2. Maximum concentration calculated with different values for the Leach Duration. Inventory and retention factors are I1R2. All runs were made with concentration boundary condition at the source (B1). Note that interpolation between different Leach duration values is not possible.
Fig 3.32-2.b Same as fig. 3.32-2.a but with source boundary condition (B2).
Fig 3.32-3.a Maximum concentration calculated with different Migration Length. Inventory and retention factors are I1R2. All runs were made with concentration boundary condition at the source (B1). Note that interpolation between different Migration Length is not possible.
Fig 3.32-3.b Same as fig. 3.32-3.a but with source boundary condition (B2).
Fig 3.33-1.a Maximum concentration calculated with different values of the Peclet Number. Inventory and retention factors are I2R1. All runs were made with concentration boundary condition at source (B1). Note that interpolation between Peclet Number values is not possible.
Fig 3.33-1.b Same as fig. 3.33-1.a but with source boundary condition (B2).
Fig 3.33-2.a Maximum concentration calculated with different values for the Leach Duration. Inventory and retention factors are I2R1. All runs were made with concentration boundary condition at the source (B1). Note that interpolation between different Leach duration values is not possible.
Fig 3.33-2.b Same as fig. 3.33-2.a but with source boundary condition (B2).
Fig 3.33-3.3b Same as fig. 3.33-3.a but with source boundary condition (B2).
Fig 3.33-3. a Maximum concentration calculated with different Migration Length. Inventory and retention factors are I2R1. All runs were made with concentration boundary condition at the source (B1). Note that interpolation between different Migration Length is not possible.
Fig 3.34-1.2 Maximum concentration calculated with different values of the Peclet Number. Inventory and retention factors are 12R2. All runs were made with concentration boundary condition at source (B1). Note that interpolation between Peclet Number values is not possible.
Fig 3.34-1.b Same as fig. 3.34-1.a but with source boundary condition (B2).
Fig 3.34-2.a Maximum concentration calculated with different values for the Leach Duration. Inventory and retention factors are I2R2. All runs were made with concentration boundary condition at the source (B1). Note that interpolation between different Leach duration values is not possible.
Fig 3.34-2.b Same as fig. 3.34-2.a but with source boundary condition (B2).
Fig 3.34-3.a Maximum concentration calculated with different Migration Length. Inventory and retention factors are I2R2. All runs were made with concentration boundary condition at the source (B1). Note that interpolation between different Migration Length is not possible.
Fig 3.34-3.b Same as fig. 3.34-3.a but with source boundary condition (B2).
SURVEY OF THE PROJECT ORGANISATION OF THE INTRACOIN STUDY AND LIST OF PARTICIPANTS

Survey of project organisation

Managing participant: SKI
Principal investigator: KEMAKTA

Coordinating group:
Chairman: Mr A Larsson, SKI
Secretary: Mr K Andersson, SKI

Project secretariat:
Mr K Andersson, SKI
Mr B Grundfelt, KEMAKTA
Mr A Bengtsson, KEMAKTA
Mr J Hadermann, EIR
Mr F Rösel, EIR
## Appendix 1:2

### List of parties participating in the INTRACOIN study, coordinating group members and project team leaders

<table>
<thead>
<tr>
<th>Party</th>
<th>Coordinating group member</th>
<th>Project team leader</th>
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<tr>
<td>Atomic Energy of Canada Ltd (AECL)</td>
<td>Mr K Dormuth</td>
<td>Mr T W Melnyk¹¹</td>
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<tr>
<td>Commissariat à l'Energie Atomique/Institut de Protection et de Sureté Nucléaire (CEA/IPSN)</td>
<td>Mr A Barbreau</td>
<td>Mr P Goblet²²</td>
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<tr>
<td>Nationale Genossenschaft für die Lagerung Radioaktiver Abfälle (NAGRA)</td>
<td>Mr C McCombie</td>
<td>Mr J Hadermann³³</td>
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<td>National Radiological Protection Board (NRPB)</td>
<td>Ms M Hill</td>
<td>Ms M Hill</td>
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<td>Projekt Sicherheitsstudien Entsorgung (PSE)</td>
<td>Mr E Bütow⁵⁵</td>
<td>Mr E Bütow⁵⁵</td>
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<tr>
<td>Technical Research Centre of Finland (VTT)</td>
<td>Mr E Peltonen⁶⁶</td>
<td>Mr E Peltonen⁶⁶</td>
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<tr>
<td>Swedish Nuclear Fuel Supply Co (SKBF/KBS)</td>
<td>Mr I Neretnieks⁷⁷</td>
<td>Mr I Neretnieks⁷⁷</td>
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<td>Swedish Nuclear Power Inspectorate (SKI)</td>
<td>Mr A Larssson</td>
<td>Mr B Grundfelt⁸⁸</td>
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<td>U.K. Atomic Energy Authority/Atomic Energy Research Establishment (UKAEA/AERE)</td>
<td>Mr D P Hodgkinson</td>
<td>Mr D P Hodgkinson</td>
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<tr>
<td>U.S. Department of Energy (U.S. DOE)</td>
<td>Mr G E Raines⁹⁹ (ONWI)</td>
<td>Mr C R Cole¹⁰¹</td>
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<td>Ms N N Finley</td>
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¹ AECL
² Ecole Nationale Supérieure des Mines de Paris
³ Swiss Federal Institute for Reactor Research
⁴ Polydynamics
⁵ Technische Universität Berlin
⁶ Mr S Vuori, VTT from 1981-06-17 to 1982-07-15
⁷ Royal Institute of Technology
⁸ KEMAKTA Consultants Co.
⁹ Mr H Burkholder, Office of Nuclear Waste Isolation from 1981-06-17 to 1982-02-19
¹⁰ Battelle Pacific Northwest Laboratory
¹¹ ONWI
¹² Intera Environmental Consultants Inc.
¹³ University of California, Berkeley
¹⁴ Geotrans Inc.
¹⁵ Sandia National Laboratories
**Appendix 1:3**

**List of abbreviations**

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<th>Abbreviation</th>
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<td>Ecole des Mines</td>
<td>Ecole Nationale Superieure des Mines de Paris, Fontainebleau, France</td>
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<td>ZIR</td>
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<td>Intera</td>
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<td>PNL</td>
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<td>TUB</td>
<td>Technische Universität Berlin, FRG</td>
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<td>UCB</td>
<td>University of California, Berkeley, Ca., U.S.A.</td>
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<td>U.S. DOE</td>
<td>Department of Energy, Washington D.C., USA</td>
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<tr>
<td>VTT</td>
<td>Technical Research Centre of Finland, Espoo, Finland</td>
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<tr>
<td>WNRE</td>
<td>Whiteshell Nuclear Research Establishment, Pinawa, Manitoba, Canada</td>
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## APPENDIX 2:1

### MODEL AND CODE CHARACTERIZATIONS

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</tr>
<tr>
<td>UCB-NE-30</td>
<td>2:112</td>
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</tbody>
</table>
Code : METIS

Project Team : Centre d'Informatique Géologique, Ecole des Mines, FONTAINEBLEAU

1) MODEL CHARACTERIZATION

1-1) Equations

1-1-1) Continuity equation for fluid

$$\nabla \cdot \dot{\mathbf{u}} = \frac{\partial}{\partial t} (c \rho) + q$$  \hspace{1cm} (1)

$$\dot{v} = - \frac{k}{\mu} \nabla (p + \rho g z) \quad \text{(Darcy's law)} \hspace{1cm} (2)$$

$$\dot{\mathbf{u}} = \dot{\mathbf{u}}(x, y, z, t)$$

$$\epsilon = \epsilon(x, y, z)$$

$$\rho = \rho(x, y, z)$$

$$q = q(x, y, z, t)$$

1-1-2) Mass balance equation for a nuclide $k$

a) Continuous medium equivalent to the fracture net :

$$\nabla (D \nabla C_k - \dot{\mathbf{u}} C_k) = \epsilon R_k \left( \frac{\partial C_k}{\partial t} + \lambda_k C_k \right) - \epsilon R_{k-1} \lambda_k C_{k-1} + A(-\rho \frac{D}{\rho} \nabla C_k) \quad (3)$$

with :

$$\mathbf{D} = \begin{bmatrix} 0 & 0 \\ 0 & a_T \end{bmatrix} \times |\mathbf{u}| + \mathbf{D}_0$$

and

$$\mathbf{D}_0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \times D_w \times \tau^2$$

in axes related to the velocity
APPENDIX 2:3

b) one dimensional equation inside the rock matrix:

\[
V \cdot (\partial C^p_p \partial_t + \nabla C^p_k) = (\epsilon_p + \rho_p K_k d_{k,k}) \left( \frac{\partial C^p_k}{\partial t} + \lambda_p C^p_k \right) - (\epsilon_p + \rho_p K_{d,k-1}) \lambda_k C^p_{k-1}
\]  

\[ (4) \]

c) Non instantaneous sorption on the surface of the fractures:

. Equation (3) becomes

\[
V \cdot (\nabla C_k - \nabla C_k) = \epsilon_p \lambda_k C_k \left( \frac{\partial C_k}{\partial t} + \lambda_k C_k - \lambda_k C_{k-1} \right) + A \phi
\]  

\[ (3 \text{ bis}) \]

where \( \phi \) is the flux exchanged between the solution and the sorbed phase.

. A second mass balance equation describes the sorbed phase:

\[
(1 - \epsilon_p) \rho_p \frac{\partial C^f_k}{\partial t} = A \phi - (1 - \epsilon_p) \rho_p \left( \lambda_k C^f_k - \lambda_k C^f_{k-1} \right)
\]  

\[ (4) \]

. The mass flux between the phases is described by a linear relationship:

\[
\phi = k_m \left( C_k - \frac{C^f_k}{K_d} \right)
\]  

\[ (5) \]

N.B : The set of equations (3 bis, 4 and 5) can represent surface sorption as well. In this case, \( C^f_k \) is a surfacic activity, \( K_d \) is replaced by \( K_m \) and \( (1 - \epsilon_p) \rho_p \) by \( A \).

d) Variation of the parameters:

\[
C_k = C_k(x, y, z, t)
\]

\[
a_L = a_L(x, y, z)
\]

\[
a_t = a_t(x, y, z)
\]

\[
D_\omega = D_\omega(x, y, z)
\]

\[
R_k = R_k(x, y, z)
\]

\[
R_{k-1} = R_{k-1}(x, y, z)
\]

\[
A = A(x, y, z)
\]

\[
D_p = D_p(x, y, z)
\]

\[
\epsilon_p = \epsilon_p(x, y, z)
\]

\[
K_a = K_a(x, y, z)
\]

\[
K_m = K_m(x, y, z)
\]

\[
K_d = K_d(x, y, z)
\]
APPENDIX 2:4

1-2) Basic assumptions

- Discrete variations of all the space dependent parameters : values defined on the elements of the finite element grid.
- 1 to 3-d laminar flow.
- No coupling between flow and transport (tracer hypothesis)
- Transport by convection and hydrodynamic dispersion. The dispersion tensor is a linear, anisotropic function of the velocity.
- Chain decay (only in 2-d version).
- Diffusion in the rock matrix treated as one dimensional, orthogonal to the fracture planes, and parallel.
- Sorption following a linear isotherm with first order kinetics.

1-3) Initial condition:

Discretized field of concentration, defined on each node and bilinearly interpolated between the nodes.

For the INTRACOM study :

\[ C_k(x, y, z, 0) = 0 \quad \forall x, y, z \]

1-4) Boundary conditions

1-4-1) Upstream

- Prescribed activity described by an arbitrary function of time : 
  \[ C_k(0, t) \quad \text{values applied at the nodes} \]
- Prescribed activity flux arbitrary function of time :
  \[ \frac{\partial C_k}{\partial x}(0, t) + vC_k(0, t) = \psi(t) \quad \text{in the 1-D cases} \]

1-4-2) Downstream

Semi infinite medium simulated with a finite grid and \( C_k(1, t) = 0 \)
\( \forall t \) at the downstream end.
APPENDIX 2:5

1-5) Restriction in parameters
\[ D \neq 0 \]

1-6) References

- P. GOBLET : Notice d'emploi du programme METIS, rapport LHM/RD/81/77, Ecole des Mines, Centre d'Informatique Géologique.

2) CODE CHARACTERIZATION

2-1) Name of code
METIS : Modélisation des Écoulements et des Transferts avec Interaction en milieu saturé (2-D version)

2-2) Method of solution
Numerical solution :
  - Bilinear finite elements
  - Central discretization in space and time
  - Diffusion in the rock matrix solved explicitly, at the end of the fracture time step.

2-3) Restriction in parameter values
  - Relationship between velocity and time step
  - Relationship between dispersivity and space discretization

2-4) Size of code and programming language
\[ \approx 5000 \text{ statements} - \text{Fortran IV} \]
APPENDIX 2:6

2-5) Applications of the code

- Heat transfer in a geothermal doublet.
- Safety analysis near surface waste storage.
- Interpretation of field tests involving non instantaneous fixation.

2-6) Availability

Subject to authorization of the Atomic Energy Committee.
APPENDIX 2:7
SWIFT MODEL AND CODE CHARACTERIZATION

1. Model characterization

1.1 Equations

Continuity equation for fluid:

\[- \nabla \cdot (\rho u) - q' = \frac{\partial}{\partial t} (\epsilon p)\]

convection production accumulation

and Darcy's law: \[u = - \frac{k}{\mu} (\nabla p - \rho g z)\]

with: \(\rho = \rho(p)\)

\[u = u(x,y,z,t)\]

\[q' = q'(x,y,z,t)\]

\[\epsilon = \epsilon(x,y,z,p)\]

\[k = k(x,y,z)\]

Continuity equation for nuclide k in a linear chain:

\[- \nabla \cdot (\rho C_k' u) + \nabla \cdot (\rho D' C_k') - q' C_k - \frac{I_k'}{\tau} + \sum_{k=1}^{K-1} \lambda_{k-1} R_{k-1}^P \epsilon \rho C_{k-1}' - \lambda_k R_k^P \epsilon \rho C_k' = \frac{\partial}{\partial t} (\epsilon \rho R_k^P C_k')\]

production dispersion production waste leach
generation decay accumulation

with: \[C_k' = C_k'(x,y,z,t)\]

\[D' = D(x,y,z)\]

\[I_k' = I_k'(x,y,z,t)\]

\[R_k^P = R_k^P(x,y,z,k)\]

Continuity equations for heat and inert component (brine) are also included in the model, but not used for INTRACOIN calculations and therefore not specified here.
APPENDIX 2:8

1.2 Assumptions

3-D, laminar flow, transient or steady state;
hydrodynamic dispersion as function of fluid velocity;
radionuclides in "tracer" quantities, i.e. nuclides
don't influence flow; linear equilibrium isotherm for
adsorption

1.3 Initial conditions

\( C'_k(x,y,z,O) = C'_{K_0}(x,y,z) \) different values for different
grid blocks possible;
used for INTRACOIN-calculations:
\( C'_k(x,y,z,O) = 0 \) for all blocks

1.4 Boundary conditions

Formulations for 1D:

1.4.1 Flow:  
- no flow : \( \frac{\partial p}{\partial x} = 0 \)
- \( p = \text{const.} : p(x_b,t) = p_b \)

1.4.2 Concentration:

a) downstream: \( \frac{\partial C'_K}{\partial x} = 0 \) no dispersive flux

b) upstream: \( u C'_K - D \frac{\partial C'_K}{\partial x} = 0 \)

1.5 Restriction in parameters
1.6 References


2. Code characterization

2.1 Name of code

SWIFT: Simulator for Waste Injection, Flow and Transport

2.2 Method of solution

Numerical solution - finite differences backward or central in space and time direct or iterative solution

2.3 Restriction in parameter values

Criteria for discretization according to finite differencing

2.4 Size of code and programming language

≈ 15 000 program statements, FORTAN IV

2.5 Computer requirements

2.5.1 Computer

CDC Cyber 175
2.5.2 **Time for one multiplication** (in seconds)

2.50E-9 s

2.5.3 **Requirements for INTRACOIN Case 1** ($T_2$, $L_1$, $I_2$, $R_1$, $P_2$)

a) Time (transport was simulated up to $2.0E+6$ years)

$1.03$ s

b) Storage

$116,000$ (oktal) words @ $40,000$ (decimal) words

2.6 **Applications of the code**

Nuclear waste isolation in geologic media
Injection of industrial wastes into saline aquifers
Determination of aquifer transport parameters from well-test data
Heat storage in aquifers
Migration of contaminants from landfills

2.7 **Availability**

*Intera Environmental Consultants Inc.*
*Houston, Texas USA*
Nomenclature

\( b \) \quad \text{boundary value index}

\( C_k \) \quad \text{concentration of nuclide } k \text{ in water} \quad (\text{kg nuclide/kg water})

\( D \) \quad \text{dispersion tensor} \quad (\text{m}^2/\text{s})

\( g \) \quad \text{acceleration due to gravity} \quad (\text{m/s}^2)

\( I_k \) \quad \text{specific inventory of nuclide } k \quad (\text{kg/m}^3 \text{ bulk})

\( K_d \) \quad \text{mass based distribution coefficient} \quad (\text{m}^3 \text{ water/kg rock})

\( K_v \) \quad \text{volume based distribution coefficient} \quad (\text{m}^3 \text{ water/m}^3 \text{ bulk})

\[ K_v = \rho K_d \]

\( k \) \quad \text{permeability tensor} \quad (\text{m}^2)

\( k \) \quad \text{nuclide index}

\( p \) \quad \text{pressure} \quad (\text{Pa})

\( q' \) \quad \text{specific rate of water withdrawal} \quad (\text{kg water} \cdot \text{m}^{-3} \text{ bulk} \cdot \text{s}^{-1})

\( R_P \) \quad \text{volume based retention factor}

\[ R_P = 1 + K_v / \varepsilon \]

\( T \) \quad \text{leaching duration} \quad (\text{s})

\( t \) \quad \text{time} \quad (\text{s})

\( u \) \quad \text{Darcy velocity of groundwater} \quad (\text{m}^3 \text{ water/m}^3 \text{ cross area} \cdot \text{s}^{-1})

\[ u = \varepsilon \cdot v \]

\( v \) \quad \text{interstitial velocity of groundwater} \quad (\text{m/s})

\( x, y, z \) \quad \text{space coordinates} \quad (\text{m})

\( Z \) \quad \text{depth below a reference plane} \quad (\text{m})

\( \varepsilon \) \quad \text{effective porosity}

\( \lambda_k \) \quad \text{decay constant of nuclide } k \quad (\text{s}^{-1})

\( \mu \) \quad \text{viscosity} \quad (\text{Pa} \cdot \text{s})

\( \rho \) \quad \text{density of water} \quad (\text{kg water/m}^3 \text{ water})

\( \rho_p \) \quad \text{bulk density of rock matrix} \quad (\text{kg rock/m}^3 \text{ bulk})
1. Model Characterization

Code: NUCDIF

1.1 Transport Equations

Continuity equation for nuclide in fissures

\[ (\frac{3}{\partial t} + \lambda) C_f(x,t) = D_L \frac{3}{\partial x^2} C_f(x,t) - \]
accumulation + decay

longitudinal dispersion

\[ -v \frac{3}{\partial x} C_f(x,t) - \frac{3(1-c_f)}{c_f r_o} N \]
advection exchange with rock blocks

Continuity equation for nuclide in rock blocks

\[ K_v (\frac{3}{\partial t} + \lambda) C_p(r,x,t) = D_p \frac{3}{\partial r^2} + \frac{\partial}{\partial r} C_p(r,x,t) \]
accumulation + decay

matrix diffusion

Coupling condition

\[ N = - D_p \frac{\partial}{\partial r} C_p(r,x,t) \bigg|_{r=r_o} \]
subscript

\[ f = \text{water in fissures} \]
\[ p = \text{water in micropores} \]

1.2 Basic assumptions

One-dimensional flow and longitudinal dispersion in fractures coupled with diffusion and instantaneous linear sorption equilibrium in spherical rock blocks.

Single decaying species.
APPENDIX 2:13

1.3 **Initial conditions**

\[ C(x,0) = C(p(x,v,0) = 0 \]

1.4 **Boundary conditions**

\[ C_f(0,t) = \begin{cases} C_0 e^{-\lambda t} & t_o \leq t \leq t_o + \Delta t \\ 0 & t < t_o, t_o + \Delta t < t \end{cases} \]

\[ C_f(\infty,t) = 0 \]

\[ \frac{\partial}{\partial t} C_p(o,x,t) = 0 \]

\[ C_p(o,x,t) = C_f(x,t) \]

1.5 **Restriction in parameters**

None

1.6 **References**


APPENDIX 2:14

2 Code characterization

2.1 Name of code

NUCDIF: NUclide DIFFusion

2.2 Method of solution

Analytical solution by Laplace transformation and inversion in the complex plane.

Numerical evaluation of resulting infinite integral by special technique.

2.3 Restriction in parameter values

None

2.4 Size of Code and Programming Language

\sim 430 program statements. FORTRAN IV

2.5 Applications of the code

Nuclear waste isolation in geologic media.

2.6 Availability

Department of Chemical Engineering, Royal Institute of Technology,
S-10044 Stockholm, Sweden.
### APPENDIX 2:15

**Nomenclature**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
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<tbody>
<tr>
<td>( C_f )</td>
<td>concentration in liquid in fissures</td>
<td>mol/m³</td>
</tr>
<tr>
<td>( C_p )</td>
<td>concentration in liquid in microfissures</td>
<td>mol/m³</td>
</tr>
<tr>
<td>( D_L )</td>
<td>longitudinal dispersion coefficient</td>
<td>m²/s</td>
</tr>
<tr>
<td>( D_{ep} )</td>
<td>effective diffusivity in micropores</td>
<td>m²/s</td>
</tr>
<tr>
<td>( K_v )</td>
<td>volume based distribution coefficient</td>
<td>m³/m³</td>
</tr>
<tr>
<td>( N )</td>
<td>molar flux from water in fissures to rock blocks</td>
<td>mol/m²s</td>
</tr>
<tr>
<td>( r )</td>
<td>radial distance from center of spherical particle</td>
<td>m</td>
</tr>
<tr>
<td>( r_o )</td>
<td>effective spherical radius</td>
<td>m</td>
</tr>
<tr>
<td>( t )</td>
<td>time</td>
<td>s</td>
</tr>
<tr>
<td>( t_o )</td>
<td>time of canister penetration</td>
<td>s</td>
</tr>
<tr>
<td>( \Delta t )</td>
<td>time for dissolution of waste</td>
<td>s</td>
</tr>
<tr>
<td>( v )</td>
<td>average velocity of water in fissures</td>
<td>m/s</td>
</tr>
<tr>
<td>( x )</td>
<td>distance in flow direction</td>
<td>m</td>
</tr>
<tr>
<td>( \varepsilon_f )</td>
<td>fracture porosity</td>
<td></td>
</tr>
<tr>
<td>( \varepsilon_p )</td>
<td>porosity of rock matrix</td>
<td></td>
</tr>
<tr>
<td>( \lambda )</td>
<td>decay constant of radionuclide</td>
<td>s⁻¹</td>
</tr>
</tbody>
</table>
APPENDIX 2:16

1. **Model Characterization**

   Code: TRUCHN

1.1 **Transport Equations**

   Continuity equation for nuclide \( k \) in a linear chain:

   \[
   \frac{\partial}{\partial t} (K^v_k C_k) = \nabla \cdot D_k \nabla C_k + \nabla \cdot v K^v_k C_k + \frac{\lambda_{k-1}}{K^v_{k-1}} C_{k-1} - \lambda_k K^v_k C_k
   \]

   with:

   \[
   C_k = C_k(x,y,z,t) \\
   D = D(x,y,z) \quad \text{1 in fissures} \\
   K^v_k = K^v_k(x,y,z,k) \text{ equal to } K^v_k \text{ in rock blocks} \\
   v = v(x,y,z)
   \]

1.2 **Basic assumptions**

   In principle 3-D fractured system and 3-D rock blocks. (However, only 1-D in rock blocks used in INTRACOIN study.) Radionuclides in "tracer" quantities, i.e. nuclides don't influence flow.

1.3 **Initial conditions**

   \[
   C_k(x,y,z,0) = C_{k_0}(x,y,z)
   \]

1.4 **Boundary conditions**

   Formulations for 1D:

   Upstream:

   \[
   C_k(o,t) = f(t)
   \]

   Downstream:

   1. Advection: \( \frac{\partial C_k}{\partial t} \)
   2. Dispersion: \( \frac{\partial C_k}{\partial x} = 0 \)
APPENDIX 2:17

1.5  **Restriction in parameters**

None

1.6  **References**


2  **Code Characterization**

2.1  **Name of code**

TRUCHN: TRUmp CHain

2.2  **Method of solution**

Numerical solution — integrated finite differences

Mixed explicit — implicit iterative scheme for advancing in the time domain.

TRUCHN modification of original TRUMP including chain decay in the discretized equations.

2.3  **Restriction in parameter values**

Criteria for discretization according to finite differencing.
APPENDIX 2:18

2.4 Size of code and programming language

~ 3 600 program statements, FORTRAN IV

2.5 Applications of the code

The original TRUMP-code and modifications have found wide applications in fluid flow problems (see for example T.N. Narasimhan: Multidimensional Numerical Simulation of Fluid Flow in Fractured Porous Media. Water Resour. Res. 18, 1235 (1982).) Nuclear waste isolation in geologic media, near and far field modeling.

2.6 Availability

Department of Chemical Engineering, Royal Institute of Technology, S-10044 Stockholm, Sweden.
APPENDIX 2:19

Nomenclature

\( C_k \) \quad \text{concentration in water of nuclide } k \quad (\text{mol/m}^3)

\( D \) \quad \text{dispersion tensor} \quad (m^2/s)

\( k_v^k \) \quad \text{volume based distribution coefficient of nuclide } k \quad (m^3/m^3)

\( k \) \quad \text{nuclide index}

\( t \) \quad \text{time (} t = 0 \text{ at start of leaching)} \quad (s)

\( v \) \quad \text{interstitial water velocity field} \quad (m/s)

\( x,y,z \) \quad \text{space coordinates} \quad (m)

\( \lambda_k \) \quad \text{decay constant of nuclide } k \quad (s^{-1})
1. Model characterization

1.1 Equations

Mass conservation equation

\[
\frac{\partial C_k}{\partial t} = D \frac{\partial^2 C_k}{\partial x^2} - v \frac{\partial C_k}{\partial x} - R_{k \rightarrow k} C_k + R_{k \rightarrow k-1} C_{k-1} 
\]

accumulation net change caused by dispersion
net change caused by convection
lost decay
generated by decay

1.2 Basic assumptions

- one-dimensional transport
- radionuclides in tracer concentrations
- homogeneous medium, laminar flow, axial dispersion
- instantaneous sorption equilibrium
- chain decay of up to 8 members including branching chains

1.3 Initial conditions

\[ C_k(x,0) = 0 \]
1.4 Boundary conditions

1.4.1 Upstream

\[ C_k(0,t) \] (time dependent concentration at inlet)

1.4.2 Downstream

\[ C_k(x,t) = 0 \] (outflow condition)

\[ x = \text{end of flow tube} \]

1.5 Restrictions to parameters

1.6 References

APPENDIX 2:22

2. Code characterization

2.1 Name of the code

MMT1D (Multicomponent Mass Transport Model in one Dimension)

2.2 Method of solution

Numerical solution (Discrete Parcel Random Walk method)

2.3 Restriction in parameter values

2.4 Size of code and programming language

~ 4700 Fortran statements. Fortran 77

2.5 Applications of the code

Safety analysis for waste repository

2.6 Availability
APPENDIX 2:23

Code: GETOUT

Project Team: Technical Research Centre of Finland, VTT

1. Model characterization

1.1 Equations

Miss conservation equation

\[ \frac{\partial C_k}{\partial t} + \frac{\partial^2 C_k}{\partial x^2} - v \frac{\partial C_k}{\partial x} = D \frac{\partial}{\partial x} \left( \frac{\partial C_k}{\partial x} \right) - R_k \lambda_k C_k + R_{k-1} \lambda_{k-1} C_{k-1} \]

- accumulation net change
- net lost caused by decay
- change caused by decay
- by dispersion
- generated by convection

1.2 Basic assumptions

- one-dimensional transport
- radionuclides in tracer concentrations
- homogeneous medium, laminar flow, axial dispersion
- instantaneous sorption equilibrium
- chain decay of up to 3 members

1.3 Initial conditions

\[ C_k(x,0) = 0 \]
APPENDIX 2:24

1.4 Boundary conditions

1.4.1 Upstream

\[ C_k(0, t) \]  \hspace{1cm} \text{(time dependent concentration at inlet)}

1.4.2 Downstream

\[ C_k(\infty, t) = 0 \]  \hspace{1cm} \text{(semiinfinite medium)}

1.5 Restrictions to parameters

\[ v > 0 \]

1.6 References

2. Code characterization

2.1 Name of the code

GETOUT

2.2 Method of solution

Analytical solution (Laplace transform technique)

2.3 Restriction in parameter values

Cases with small Peclet number cause trouble

2.4 Size of code and programming language

~ 3800 Fortran statements. Fortran IV

2.5 Applications of the code

Safety analysis for waste repository

2.6 Availability
APPENDIX 2:26

Code: SWENT
Project Team: INTERA Environmental Consultants, Inc.
Houston, Texas USA

1 MODEL CHARACTERIZATION

This code calculates the transient three-dimensional transport of fluid, energy, a dominant inert contaminant and a number of radionuclides. Each of these transport processes is described by a conservation equation. The first three equations are coupled by the fluid properties, density and viscosity. The velocity field is obtained from the solution of the first three coupled equations and is used in the solution of the fourth equation. Radionuclides are assumed to be present in trace quantities only; and therefore, have no effect on the velocity. These equations are uncoupled from the first three.

1.1 EQUATIONS

Flow Equation

Suppose x,y,z to be a Cartesian coordinate system with the positive direction of the z-axis being vertically downward. Then, the basic equation single-phase flow in a porous medium results from a combination of the continuity equation

\[-\nabla \cdot (\rho u) - q' = \frac{\partial}{\partial t} (\phi p)\]  

\[-\text{net sink/source* accumulation}\]

and Darcy's law in three dimensions:

\[u = -\frac{k}{\mu} (\nabla p - \rho g \nabla z)\]  

By the convention adopted here, \(q' > 0\) is a sink term and \(q' < 0\) is a source term.
where: $g =$ acceleration due to gravity

$k$ = permeability tensor

$p =$ fluid pressure

$q' =$ fluid discharge rate

$u =$ Darcy velocity vector

$\rho =$ fluid density

$\mu =$ fluid viscosity

$\phi =$ porosity

The result is the basic flow equation for fluid pressure:

$$V \cdot \rho \left[ \frac{k}{\mu} (Vp - \rho g z) \right] - q' = \frac{\partial}{\partial t} (\phi p) \quad (1-3)$$

**Nuclide Transport Equation**

A material balance for $N$ radioactive components results in $N$ component equations:

$$-V \cdot (\rho C_i u) + V \cdot (\rho E_{i} \cdot V C_i) - q_i - q_i C_i$$

Net component $i$ convection of component $i$ Sink/Source Sink/Source with no fluid accompaniment injection, efflux/ influx

$$+ \sum_{j=1}^{N} k_{ij} \lambda_{j} \phi p C_{j} - \lambda R_{i} \phi p C_{i} = \frac{\partial}{\partial t} (\phi R_{i} C_{i}) \quad (1-4)$$

Generation of Net decay of Accumulation component $i$ by component $i$ to other isotopes isopotes

where: $E =$ dispersivity tensor

$k_{ij} =$ mass fraction of component $j$ decaying to component $i$

$R_{i} =$ retardation factor

$\lambda_{j} =$ decay rate of component $i$

Continuity equations for heat and inert component (brine) are also included in the model, but are not presented here since they were not used for INTRACOIN.
The fluid properties and other parameters used in the Equations (1-1) to (1-4) are assumed to be given by the following relations (Muller et al, 1981). For INTRACOIN, there are only trace concentrations of radionuclides and an inert solute is not present, hence $C$ is zero in the equations given below.

**Fluid Density**

$$\rho = \rho_o \left[ 1 + C_w (p-p_o) - C_T (T-T_o) + C_s \bar{C} \right]$$  \hspace{1cm} (1-5)

where:  
- $C_w$ = fluid compressibility  
- $C_T$ = coefficient of thermal expansion of fluid  
- $C_s = \frac{\rho(p_o, T_o, \bar{C}=1) - \rho(p_o, T_o, \bar{C}=0)}{\rho(p_o, T_o, \bar{C}=0)}$  \hspace{1cm} (1-6)

**Fluid Viscosity**

$$\mu = \mu_R(\bar{C}) \exp \left[ B(\bar{C}) \left( T^{-1} - T_R^{-1} \right) \right]$$  \hspace{1cm} (1-7)

where $\mu_R$ and $T_R$ are reference viscosity and temperature, respectively.

**Porosity**

$$\phi = \phi_o \left[ 1 + C_r (p-p_o) \right]$$  \hspace{1cm} (1-8)

where:  
- $C_r$ = rock compressibility
APPENDIX 2:29

Dispersion Tensor

The constituent dispersion tensor, $E$, is taken in the present model as dependent upon the hydrodynamic dispersivity. This dispersivity is a function of the local fluid velocity.

The general expression for the constituent dispersion, $E$, in terms of $D_m$ (molecular diffusivity), as well as hydrodynamic dispersivity $D$, can be written as:

$$E = D + D_m I$$

(1-9)

where $I$ is the identity matrix and where the elements of $D_m$, assuming the medium to be isotropic, are given by:

$$D_{ij} = \alpha_L \frac{u_i u_j}{|u|} + (\alpha_L - \alpha_T) \frac{u_i u_j}{|u|}$$

(1-10)

where the $\alpha_L$ and $\alpha_T$ refer to longitudinal and transverse dispersivities, respectively.

Adsorption Isotherm

A linear equilibrium adsorption isotherm is used to give the retardation factor $R_i$ (Equation 1-4) in terms of the distribution coefficient $K_{di}$ as:

$$R_i = 1 + K_{di} \frac{(1-\phi)\rho}{\phi}$$

(1-11)

1.2 BASIC ASSUMPTIONS

- 3-D, transient or steady-state transport.
- Only a single liquid phase exists.
- Porous medium is saturated with the fluid.
- Flow is laminar and governed by Darcy's Law.
- Fluid viscosity is an exponential function of temperature.
- Linear equilibrium isotherm for adsorption.
APPENDIX 2:30

- Hydrodynamic dispersion is a linear function of velocity.
- Effects of hydrodynamic dispersion and molecular diffusivity are additive.

1.3 INITIAL CONDITIONS

Table 1-1 shows the types of initial conditions accepted by the model. For INTRACOIN, a steady-state flow field is first established and the initial concentration of radionuclides is assumed to be zero throughout the system.

\[ C_i(x,v,z,0) = 0 \text{ for all blocks.} \]

1.4 BOUNDARY CONDITIONS

This model permits the implementation of all the three standard types of boundary conditions (B.C.) with the partial differential equations. They are:

1. Dirichlet B.C. (Type 1)
2. Neumann B.C. (Type 2)
3. Cauchy B.C. (Type 3)

The boundary conditions may be time-independent or time-dependent. Table 1-2 shows the boundary conditions handled by the partial differential equations for pressure and trace component concentration. If no boundary condition is specified at the edges of the finite-difference grid, a zero flux condition will be implied.

For INTRACOIN applications, the boundary conditions are expressed mathematically as follows.

1.4.1 Flow

Uniform flow conditions were described by specifying pressures at the two boundaries - inlet and outlet.

\[ p(0,t) = p_o \]
\[ p(L,t) = p_L \]
## Table 1-1. Initial Conditions

<table>
<thead>
<tr>
<th>Variable</th>
<th>Initial Conditions</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure</td>
<td>Hydrostatic Distribution</td>
<td>The pressure, at any chosen reference point, is input by the user. The model imposes the same hydraulic potential throughout the system.</td>
</tr>
<tr>
<td>Temperature</td>
<td>A function of depth only.</td>
<td>User can input as many values of temperature and $z$ as required, including the overburden and underburden, to define the geothermal gradient.</td>
</tr>
<tr>
<td>Trace Comp.</td>
<td>Function of spatial Co-ordinates</td>
<td>Initial concentrations in each grid block can be specified.</td>
</tr>
<tr>
<td>Concentration</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>


APPENDIX 2:32

1.4.2 Concentration

a) Upstream

B2: Incorporation of source term $I_1(t) \delta(x) / \text{FT}$ within the transport equation ($\delta(x)$ is the Dirac delta function) and accordingly

$$\frac{\partial c}{\partial x} = 0 \text{ at } x = 0$$

Since the source block was the first block in the finite-difference formulation, this condition is identical to

$$uC_o - uC_{x=0} - \frac{\partial C}{\partial x}_{x=0}$$

b) Downstream

F1 : $C_1(+w, t) = 0$

This condition was simulated by using the system length of 800 m, and specifying $E_3$ condition at 800 m.

$$E3 : \frac{\partial}{\partial x} C_1(L, t) = 0$$

1.5 RESTRICTION IN PARAMETERS

None.
<table>
<thead>
<tr>
<th>Variable</th>
<th>Type of B.C.</th>
<th>Time-Dependent/ Constant</th>
<th>Designation for Blocks with B.C.</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure</td>
<td>Dirichlet (Type 1)</td>
<td>Constant</td>
<td>Boundary grid blocks</td>
<td>These blocks are at the edge of the finite-difference grid and specify the conditions imposed by the surroundings such as rivers, lakes, etc. If the user does not specify any B.C. at the edges of the grid, zero flux will be imposed.</td>
</tr>
<tr>
<td>Water Flux</td>
<td>Neumann (Type 2)</td>
<td>Constant or Time-Dependent</td>
<td>Well Blocks</td>
<td>These B.C. may be specified either at the bottom-hole or at the well head. In the latter case, a wellbore model calculates the corresponding values in the grid block.</td>
</tr>
<tr>
<td>Pressure</td>
<td>Neumann</td>
<td>Constant</td>
<td>Top layer of grid blocks only</td>
<td></td>
</tr>
<tr>
<td>Vertical Recharge</td>
<td>Neumann (Type 2)</td>
<td>Constant or Time-Dependent</td>
<td>Top layer of grid blocks only</td>
<td></td>
</tr>
<tr>
<td>Variable</td>
<td>Type of B.C.</td>
<td>Time-Dependent/ Constant</td>
<td>Designation for Blocks with B.C.</td>
<td>Remarks</td>
</tr>
<tr>
<td>-----------------</td>
<td>-------------------</td>
<td>--------------------------</td>
<td>----------------------------------</td>
<td>--------------------------------------------------------------------------</td>
</tr>
<tr>
<td>Trace Cauchy</td>
<td>Time-Dependent</td>
<td>Source Blocks</td>
<td>These source blocks can handle the fluxes of radioactive components, water, and heat. (Designated as B2 for INTRACOIN)</td>
<td></td>
</tr>
<tr>
<td>(Radioactive)</td>
<td>or Constant</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Component Flux</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>for each</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>component*</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water Flux</td>
<td>Neumann</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Normal Derivatives of Trace Comp. Conc.</td>
<td>Zero Value</td>
<td>Efflux Blocks</td>
<td>Model assumes no dispersion at the efflux blocks.</td>
<td></td>
</tr>
</tbody>
</table>

* This value may be obtained from a near-field repository model or from the waste leach submodel in SWENT.
APPENDIX 2:35

1.6 REFERENCES


APPENDIX 2:36

2 CODE CHARACTERIZATION

2.1 NAME OF CODE

SVENT: Simulator of Waste, Energy and Nuclide Transport

2.2 METHOD OF SOLUTION

Numerical finite difference

- backward or centered in space and time
- reduced band-width direct or two-line successive overrelaxation (L2SOR) solution

2.3 RESTRICTION IN PARAMETER VALUES

The space and time discretization criteria are shown in Table 2-1.

2.4 SIZE OF CODE AND PROGRAMMING LANGUAGE

14,600 lines in FORTRAN IV.

2.5 APPLICATIONS OF THE CODE

- Nuclear waste isolation in geologic media
- Injection of industrial wastes into saline aquifers
- Determination of aquifer transport parameters from well-test data
- Heat storage in aquifers
- Migration of contaminants from landfills

2.6 AVAILABILITY

INTERA Environmental Consultants, Inc.
Houston, Texas U.S.A.
Table 2-1. Numerical Criteria for Radionuclide Transport

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Numerical Dispersion</th>
<th>Dispersion Overshoot</th>
<th>Criteria</th>
</tr>
</thead>
<tbody>
<tr>
<td>CIT-CIS</td>
<td>None</td>
<td>None</td>
<td>$v\Delta t/\Delta x + 2D'\Delta t/\Delta x^2 &lt; 1$; $v\Delta x/2 &lt; D'$</td>
</tr>
<tr>
<td>CIT-BIS</td>
<td>$v\Delta x/2$</td>
<td>$v\Delta x/2 &lt; D'$</td>
<td>$v\Delta t/\Delta x + 2D'\Delta t/\Delta x^2 &lt; 1$</td>
</tr>
<tr>
<td>BIT-CIS</td>
<td>$v^2\Delta t/2$</td>
<td>$v^2\Delta t/2 &lt; D$</td>
<td>$v\Delta x/2 &lt; D'$</td>
</tr>
<tr>
<td>BIT-BIS</td>
<td>$v\Delta x/2 + v^2\Delta t/2$</td>
<td>$v\Delta x/2 + v^2\Delta t/2 &lt; D'$</td>
<td>None</td>
</tr>
</tbody>
</table>

* Here CIT means central-in-time, CIS means central-in-space, BIT refers to backward-in-time, and BIS refers to backward-in-space.

Definition of terms:

- $R = 1 + (1-\phi)\rho_t k_d / \Phi$
- $v = \frac{u}{\Phi R}$
- $(\alpha_L u + D_m )/R\phi$

where

- $v$ = interstitial velocity
- $D_m$ = molecular diffusivity
APPENDIX 2:38

Code: FTRANS
Project Team: INTERA Environmental Consultants, Inc.
Houston, Texas USA

1 MODEL CHARACTERIZATION

1.1 EQUATIONS

1.1.1 Fluid Flow

(A) Dual-Porosity System

\[
\frac{\partial}{\partial x_i} \left( T_{ij} \frac{\partial h}{\partial x_j} \right) = S \frac{\partial h}{\partial t} - \Lambda - q \quad i, j = 1, 2
\]

\( h \) = hydraulic head in the fracture

\( T_{ij} \) = transmissivity tensor of formation

\( S \) = formation storage coefficient

\( \Lambda \) = volumetric rate of fluid transfer per unit area from porous matrix blocks to fractures

\( q \) = volumetric rate of fluid flow per unit area via sources (or sinks)

\( x_i, x_j \) = co-ordinate axes in plane of fracture

\( t \) = time

(R) Single-Continuum System

\[
\frac{\partial}{\partial x_i} \left( \kappa_{ij} \frac{\partial h}{\partial x_j} \right) = S \frac{\partial h}{\partial t} - q
\]

\( \kappa_{ij} \) = continuum hydraulic conductivity tensor

\( S_s \) = coefficient of specific storage of continuum
1.1.2 Solute Transport

(A) Fracture Transport

\[ \frac{3}{\delta x_1} \left( D_{ij} \frac{3C_k}{\delta x_j} \right) - \nu_i \frac{3C_k}{\delta x_i} = \frac{3}{\delta t} \left( \phi R_{k, k} \right) + \phi R_{k, k} \frac{3C_k}{\delta x_1} \]

\[ - \sum_{m=1}^{M} \xi_{km} \phi R_m \lambda C_m - q \left( C_k^* - C_k \right) - \Gamma_k \]

\( x_1, x_2 = \) co-ordinate axes in plane of fracture

\( C_k = \) trace fluid concentration of component \( k \)

\( D_{ij} = \) hydrodynamic dispersion tensor

\( \nu_i = \) Darcy velocity vector in fracture

\( \phi = \) effective fracture porosity (equals 1.0 if no deposition and fracture is completely filled with fluid)

\( \lambda_k = \) first-order decay constant of component \( k \)

\( R_k = \) retardation factor for component \( k \)

\( \xi_{km} = \) fraction of parent component \( m \) decaying into component \( k \)

\( M = \) number of parents decaying to component \( k \)

\( R_{m, k, m} C_m = \) retardation factor, decay constant and fluid concentration of \( m \)th parent component

\( q = \) rate of fluid injection via sources (e.g., wells)

\( C_k^* = \) concentration of \( k \) in injected fluid

\( \Gamma_k = \) rate of material transfer of \( k \) from rock matrix to fracture

(B) Matrix Transport (no advection)

- Rectangular blocks [Figure 1-1 (a)]

\[ \frac{3}{\delta z} \left( D' \frac{3C'_k}{\delta z} \right) = \frac{3}{\delta t} \left( \phi R'_k C'_k \right) + \phi R'_k \lambda_k C'_k - \sum_{m=1}^{M} \xi_{km} \phi R'_m \lambda C'_m \]

- Spherical blocks [Figure 1-1 (b)]

\[ \frac{n'}{r^2} \frac{3}{\delta r} \left( r^2 \frac{3C'_k}{\delta r} \right) = \frac{3}{\delta t} \left( \phi R'_k C'_k \right) + \phi R'_k \lambda_k C'_k - \sum_{m=1}^{M} \xi_{km} \phi R'_m \lambda C'_m \]
Figure 1-1. Typical Matrix Block Fracture Units: (a) Rectangular Prismatic Block Representation and (b) Spherical Matrix Block Representation
APPENDIX 2:41

z = co-ordinate perpendicular to fracture plane and along thickness of rectangular block

r = radial distance from center of physical block

\( D' = \) coefficient of molecular diffusion (all primes denote properties that refer to the porous matrix blocks)

\[ (C) \text{ Fracture-Matrix Coupling Term} \]

\[ \Gamma_k = (D' \frac{\partial C'}{\partial z} \bigg|_{z=0}) \left( \frac{1 - \epsilon_f}{\epsilon_f} \right) \sigma. \]

\[ \epsilon_f = \text{fractures (secondary) porosity} = \frac{\text{volume of fractures}}{\text{volume of entire medium}} \]

\[ \sigma = \text{surface to volume ratio of block} \]

1.2 BASIC ASSUMPTIONS AND LIMITATIONS

1.2.1 Flow Model

Assumptions

1. Flow in the rock matrix and fractures obeys Darcy's law.
2. The porous medium reservoir is confined by impermeable overlying and underlying formations.
3. For fractured reservoir systems, the aperture of the fractures is assumed to be very small compared with other dimensions in the fracture plane.
4. Boundary conditions are assumed to be invariant with time.
1.2.2 Solute Transport Model

Assumptions

1. The hydrodynamic dispersion is defined as the sum of the coefficients of mechanical dispersion and molecular diffusion. The medium dispersivity is assumed to correspond to that of an isotropic porous medium and hence related to two constants \( \epsilon_L \) and \( \epsilon_T \), which are the longitudinal and transverse dispersivities.

2. The velocity field used in the advective-dispersive transport equation is assumed to be in a steady-state condition.

3. The adsorption and decay of the radionuclides are described by a linear equilibrium isotherm and a set of first-order decay constants, respectively.

4. For fractured medium systems, the aperture of the fracture is assumed to be small compared with other dimensions in the fracture plane. Flow and transport in each fracture are along the fracture plane.

5. In the dual-porosity idealization of the fractured porous medium system, all porous blocks are assumed to have the same set of properties.

Limitations

1. The model cannot simulate the kinetic adsorption between the fluid and liquid phases.

2. The model requires the knowledge of geometry of fractures. Such knowledge includes information pertaining to fracture apertures and fracture spacing. This type of information may not be readily available.

3. The model cannot simulate fully three-dimensional transport. The current version of the code only permits the user to employ rectangular finite elements in the discretization of a two-dimensional domain.

4. For the case of fractured system with substantially permeable rock matrix, the model can only simulate one-dimensional (or radial)
advective-dispersive transport in the line fractures and two-dimensional (or axisymmetric) advective-dispersive transport in the porous matrix.

1.3 INITIAL CONDITIONS

1.3.1 Flow Model

\[ h(x_1, x_2, t = 0) = h_0(x_1, x_2) \]

1.3.2 Solute Transport Model

\[ C_k = (x_1, x_2, t = 0) = C_k^0(x_1, x_2) \]

\[ h_0 = \text{initial head in fracture plane} \]
\[ c_k^0 = \text{initial concentration in fracture plane} \]

1.4 BOUNDARY CONDITIONS

1.4.1 Flow Model

\[ h = \bar{h} \quad \text{... on } B_1 \]
\[ - \frac{T}{\eta_j} \frac{\partial h}{\partial x_j} n_i = \bar{q} \quad \text{... on } B_2 \]

\[ B_1 = \text{boundary whose hydraulic head, } \bar{h}, \text{ is specified.} \]
\[ B_2 = \text{boundary where fluid flux, } \bar{q}, \text{ is specified.} \]

1.4.2 Solute Transport Model

(A) Fracture

\[ C_k = \bar{c}_k(t) \quad \text{on } B_1 \]
\[ v_i n_i C_k - (D_{ij} \frac{\partial C_k}{\partial x_j}) n_i - \bar{q} \bar{c}_k(t) \quad \text{on } B_2 \]
$
\tilde{C}_k = \text{prescribed concentration along boundary } B_1$
$q \tilde{C}_k = \text{prescribed flux describing total outward material flux along boundary, } B_2$
$n_1 = \text{outward unit normal vector on } B_2$

$\tilde{T}_k(t)$, the inventory, satisfies Bateman's equations of first-order
generation and decay.

$$
\frac{d\tilde{T}_k}{dt} = -\lambda_k \tilde{T}_k + \sum_{m=1}^{M} \xi_{km} \lambda_m \tilde{T}_m
$$

$\tilde{C}_k(t) = \frac{I_k(t)}{AT}$ on $B_1$

and

$q \tilde{C}_k = \frac{I_k(t)}{AT}$ on $B_2$

$A = \text{inlet cross-section area}$
$\tau = \text{leach time}$

(R) Matrix

- Rectangular [Figure 1-1 (a)]

$C_k'(z=0, x_1, x_2, t) = C_k(x_1, x_2)$

$C_k'(z=b', x_1, x_2, t) = C_k(x_1, x_2)$

- Spherical [Figure 1-1 (b)]

$C_k'(r=a, x_1, x_2, t) = C_k(x_1, x_2)$

$\lim_{r \to 0} (rC_k') = 0$

$b' = \text{thickness of rectangular block}$
$a = \text{radius of spherical block}$
$C_k' = \text{matrix concentration}$
$C_k = \text{fracture concentration}$
1.5 RESTRICTION IN PARAMETER VALUES

None

1.6 REFERENCES

APPENDIX 2:46

2 CODE CHARACTERIZATION

2.1 NAME OF CODE

FTRANS - 2-D Code for Fluid Flow and Transport of Radioactive Nuclides in Fractured Rock

2.2 METHOD OF SOLUTION

Numerical, finite-elements using upstream-weighted residuals.

2.3 RESTRICTION IN PARAMETER VALUES

\[ Pe = \frac{\text{Element size}}{\text{Dispersivity}} \leq 2 \]

\[ \Delta t \leq 0.5 \times \text{Minimum half-life}. \]

2.4 SIZE OF CODE AND PROGRAMMING LANGUAGE

2090 program lines, FORTRAN IV

2.5 POTENTIAL APPLICATIONS OF THE CODE

- Fractured, porous media flow and radionuclide transport in repository performance assessment
  - Near-field
  - Far-field

- Problems involving the evaluation of pumping and tracer test data to determine the hydraulic and transport properties of fractured/porous formations

2.6 AVAILABILITY

INTERA Environmental Consultants, Inc.
Houston, Texas USA
APPENDIX 2:47

FORMAT FOR MODEL AND CODE CHARACTERIZATION

1. Model Characterization

Codes RANCH (a)

CONZRA/RANCH (b)

Swiss Federal Institute for Reactor Research

CH-5303 Würenlingen

Switzerland

\[
\begin{align*}
\text{a)} \quad & R_k \left( \frac{\partial}{\partial t} + \lambda_k \right) C_k(x,t) = D \frac{\partial^2}{\partial x^2} C_k(x,t) - \frac{\partial}{\partial x} C_k(x,t) + R_{k-1} \lambda_k C_{k-1}(x,t) \\
\text{b)} \quad & R_k \left( \frac{\partial}{\partial t} + \lambda_k \right) C_k(x,t) = D \frac{\partial^2}{\partial x^2} C_k(x,t) - \frac{\partial}{\partial x} C_k(x,t) + R_{k-1} \lambda_k C_{k-1}(x,t) + \frac{F_k(t)}{F} \delta(x)
\end{align*}
\]

1.2 Basic assumptions

one-dimensional transport
layered medium with piecewise constant parameters
instantaneous linear sorption equilibrium

1.3 Initial conditions

\[ C_k(x,0) = 0 \]
APPENDIX 2:48

1.4 **Boundary conditions**

1.4.1 **Upstream**

a) $C_k(0,t)$ arbitrary time dependent concentration at inlet (Dirichlet boundary)

b) $F_k(t)$ arbitrary plane source injection rate

$C_k(-\infty,t) = 0$ infinite medium

1.4.2 **Downstream**

$C_k(\infty,t) = 0$ semi infinite medium

1.5 **Restriction in parameters**

$a^i_1 << 1$

1.6 **References**


- J. Hadermann and J. Patry, Nucl. Technol. 54 (1981) 266

2. Code Characterization

2.1 Name of code

RANCH, CONZRA

2.2 Method of solution

Semi-analytical solution: Laplace transformation

2.3 Restriction in parameter values

1. \( k < 4 \)
2. \( i < 10 \)
3. \( a^i/n^i < .4 \)

2.4 Size of Code and Programming Language

RANCH: 1000 program statements
CONZRA: 800 program statements

CDC Fortran extended FTN 4.8
CDC Compass 3.6

2.5 Applications of the code

Migration of radionuclides from deep-lying repository sites in northern Switzerland (e.g. Berlin conference, June 1982)

2.6 Availability

Swiss Federal Institute for Reactor Research and National Cooperative for the Storage of Radioactive Waste
NOMENCLATURE

Space and time dependencies of quantities are not explicitly given.

- \( a^i \): longitudinal dispersion length \( [m] \)
- \( C_k \): concentration in water of nuclide \( k \) \( [Ci/m^3 \text{ water}] \)
- \( D^i \): dispersion tensor \( [m^2/s] \)
- \( F \): cross section for flow of contaminated water at inlet \( [m^2] \)
- \( F_k \): injection rate at geosphere inlet for nuclide \( k \) \( [Ci/s] \)
- \( i \): index of layer
- \( k \): nuclide index
- \( l_i \): migration length in layer \( i \)
- \( R_k^i \): retention factor for nuclide \( k \)
- \( t \): time (\( t=0 \) at start of leaching) \( [s] \)
- \( v^i \): interstitial water velocity \( [m/s] \)
- \( x \): space coordinate \( [m] \)
- \( \delta(x) \): Dirac delta function
- \( \lambda_k \): decay constant of nuclide \( k \) \( [s^{-1}] \)
APPENDIX 2:51

FORMAT FOR MODEL AND CODE CHARACTERIZATION

1. Model Characterization

Code RANCHN

Swiss Federal Institute for Reactor Research
CH-5303 Würenlingen
Switzerland

\[
\frac{\partial}{\partial t} C_k(x,t) = f(x,t,C_k) - \frac{\partial^2}{\partial x^2} C_k(x,t) - g(x,t,C_k) \frac{\partial}{\partial x} C_k(x,t) +
\]

\[+ h(x,t,C_k)\]

1.2 Basic assumptions

one-dimensional transport

1.3 Initial conditions

\[C_k(x,0) \text{ any given function}\]

1.4 Boundary conditions

any boundary condition of the form

\[
\alpha_u C_k(0,t) + \beta_u \frac{\partial C_k(x,t)}{\partial x} \bigg|_{x=0} = \gamma_k u
\]
1.4.2 Downstream

\[ a_d k C_k(x,d,t) + \beta_d k \frac{\partial C_k(x,t)}{\partial x} \bigg|_{x=x_d} = \gamma_d \]

1.5 Restriction in parameters

No restriction

1.6 References

F. Rösel and J. Hadermann, EIR-Internal Reports

2. Code Characterization

2.1 Name of code

RANCHN

2.2 Method of solution

Spectral method in space
Gear method in time

2.3 Restriction in parameter values

No restriction

2.4 Size of Code and Programming Language

800 program statements
CDC Fortran extended FTN 4.8
APPENDIX 2:53

2.5 Applications of the code

Migration of radionuclides from deep-lying repository sites in northern Switzerland

2.6 Availability

Swiss Federal Institute for Reactor Research and National Cooperative for the Storage of Radioactive Waste

NOMENCLATURE

Space and time dependencies of quantities are not explicitly given.

\( C_k \) concentration in water of nuclide \( k \) [Ci/m\(^3\) water]

\( k \) nuclide index

\( t \) time (\( t=0 \) at start of leaching) [s]

\( x \) space coordinate [m]

\( \lambda_k \) decay constant of nuclide \( k \) [s\(^{-1}\)]

\( f(x,t) \) \( g(x,t) \) \( h(x,t) \) any given function of \( x \) and \( t \); they may also depend on \( C(x,t) \)

\( \alpha_u, \beta_u, \gamma_u \) \( \alpha_d, \beta_d, \gamma_d \) constants for the upstream and downstream boundary conditions

\( x_d \) coordinate of the downstream b.c.
Code: GEOS


1. Model Characterisation

1.1 Transport Equation

For INTRACOIN Level 1, Cases 1, 2 and 3:

\[
R_k \left( \frac{\partial}{\partial t} + \lambda_k \right) C_k = D \frac{\partial^2}{\partial x^2} C_k - \frac{\partial}{\partial x} V C_k
+ R_{k-1} \lambda_k C_{k-1} + \frac{F_k}{F} \delta(x)
\]

where \( C_k = C_k(x,t) \)
\( F_k = F_k(t) \)
\( R_k = R_k(x) \) [piecewise constant or linear function]
\( D = D(x) \) [piecewise constant]

For INTRACOIN Level 1, Case 7:

\[
\epsilon \left( \frac{\partial}{\partial t} + \lambda_k \right) C_k = \epsilon D \frac{\partial^2}{\partial x^2} C_k - \epsilon V \frac{\partial}{\partial x} C_k + \epsilon \lambda_k C_{k-1}
- k_\text{m} A(C_k - \frac{C_p^k}{k_{\text{d}}}) + \frac{F_k}{F} \delta(x)
\]

\[
\rho_p \left( \frac{\partial}{\partial t} + \lambda_k \right) C_k^p = \rho_p \lambda_k C_{k-1}^p + k_\text{m} A(C_k - \frac{C_k^p}{k_{\text{d}}})
\]

where \( C_k = C_k(x,t) \)
\( C_k^p = C_k^p(x,t) \)
\( F_k = F_k(t) \)

1.2 Basic Assumptions

One-dimensional transport.

Groundwater velocity constant in space and time.

Instantaneous linear equilibrium sorption for cases 1, 2 and 3.

Linear chain decay.

Arbitrarily time dependent injection source.
APPENDIX 2:55

1.3 Initial Conditions
\[ C_k(x, 0) = 0; \quad C^p_k(x, 0) = 0. \]

1.4 Boundary Conditions

1.4.1 Upstream
\[ C_k(x < 0, t) = 0; \quad C^p_k(x < 0, t) = 0. \]
No flow across the \( x = 0 \) boundary.
Time dependent radionuclide injection source.

1.4.2 Downstream
\[ C_k(x_0, t) = C^p_k(x_0, t) = 0. \]
Concentration boundary at \( x = x_0 \).

1.5 Restriction in parameters

1.6 References

2. Code Characterisation

2.1 Name of code
GEOS

2.2 Method of solution
Numerical solution: Finite difference
Backward in space
Gear's method in time

2.3 Restriction in parameter values
Maximum of 9 radionuclides.
Numerical dispersion imposes minimum number of space steps.
Maximum number of space steps is limited by the FACSIMILE program.

2.4 Size of code and programming language
About 300 program statements. FACSIMILE.
APPENDIX 2:56

2.5 Applications of the code


Generic radiological assessment of a high-level waste repository.


Sensitivity analysis.


2.6 Availability

Contact: M. D. Hill, National Radiological Protection Board, Chilton, Didcot, Oxfordshire OX11 ORQ, England.
APPENDIX 2:57

Code: TROUGH-ID

Project Team: Polydynamics Limited

1. MODEL CHARACTERISATION

1.1 Transport Equations

a) Cases 1 and 2: Nuclide transport equation with linear sorption equilibrium

\[
\frac{3}{3t} [R_k \varepsilon N_k] = \frac{3}{3x} [D_k \frac{3}{3x} \varepsilon N_k] - \frac{3}{3x} [V \varepsilon N_k] + \lambda_{k-1} R_k \varepsilon N_{k-1} - \lambda_k R_k \varepsilon N_k
\]

where:

\[N_k = N_k(x,t)\]
\[D_k = D_k(x)\]
\[R_k = R_k(x,k)\]
\[\varepsilon = \varepsilon(x)\]

b) Case 7: Nuclide transport equations with non-equilibrium sorption.

The fluid equation:

\[
\frac{3}{3t} [\varepsilon N_k] = \frac{3}{3x} [D_k \frac{3}{3x} \varepsilon N_k] - \frac{3}{3x} [V \varepsilon N_k] + \lambda_{k-1} \varepsilon N_{k-1} - \lambda_k \varepsilon N_k
\]

\[- AK_m \left[(R_k - 1) \varepsilon N_k - (1 - \varepsilon) C'\right]\]
The associated equation for the conservation of the nuclide immobilised in the solid is:

\[
\frac{3}{\partial t} [(1-\varepsilon) C'_k] = \lambda_{k-1}(1-\varepsilon) C'_{k-1} - \lambda_k(1-\varepsilon) C'_k + AK_m [(R_{k-1}) \varepsilon N_k - (1-\varepsilon) C'_k]
\]

where:

\[C'_k = C'_k(x,t)\]

1.2 Basic Assumptions

- one-dimensional transport
- 1-D steady state flow
- radionuclides in "tracer" quantities, i.e. nuclides do not influence flow
- instantaneous linear sorption equilibrium for cases 1 and 2
- reversible sorption kinetics for case 7

1.3 Initial Conditions

\[N_k(x,0) = 0\]
\[C'_k(x,0) = 0\]

1.4 Boundary Conditions

B1

- \(x_u = 0\)
- \(\alpha_u = 1.0\)
- \(\beta_u = 0\)
- \(\gamma_u = I_k(t) / \nu c PT\)

B2

- \(x_u = \) not used
- \(\alpha_u = \) not used
- \(\beta_u = \) not used
- \(\gamma_u = \)
Appendix 2:59

E1

\[ x_d = 2.5 \text{ km} \]
\[ a_d = 1.0 \]
\[ \beta_d = 0 \]
\[ \gamma_d = 0 \]

E2

\[ x_d = \]
\[ a_d = \]
\[ \beta_d = \text{not used} \]
\[ \gamma_d = \]

E3

\[ x_d = \]
\[ a_d = \]
\[ \beta_d = \text{not used} \]
\[ \gamma_d = \]

1.4.1 Upstream

\( C_k(0,t) \) time dependent concentration at the inlet boundary corresponding to the exact solution of the Bateman equations. Over each time step the integral mean value of this exact solution is used to define the time-discretised leaching rate.

1.4.2 Downstream

\( C_k(\omega,t) = 0 \) semi-infinite medium, simulated by adding at least 1 km to the downstream end of the domain of interest and fixing the concentration to zero at this point.

1.5 Restriction in parameters

1.6 References

TROUGH-1D User Manual
2. CODE CHARACTERISATION

2.1 Name of Code

TROUGH: Transport of Radionuclide Outflows in Underground Hydrology

2.2 Method of Solution

Numerical solution:

- finite differences (1st order)
- hybrid in space and forward in time
- fully or partially implicit, direct or iterative solution

2.3 Restriction in Parameter Values

- \( \lambda, V, K_m \neq 0 \)

- Maximum cell size not greater than half of the minimum dispersion length in the domain to maintain accuracy. If \( D = 0 \) explicit time differencing must be used and time steps become cell-size dependent.

2.4 Size of Code and Programming Language

662 program statements; FORTRAN IV extended (CDC).

2.5 Application of the Code

TROUGH-1D was written for NAGRA (CH) to study far field migration problems in porous and fissured media and to serve as a test bed for multidimensional versions. The processes which can be treated with the code are:

- transport of nuclides or other chemicals by convection
- nuclide retention, with chemical equilibrium
- nuclide retention, with kinetic domination
- diffusion of nuclides into the microfissures of the solid matrix

2.6 Availability

The program is available at Polydynamics Limited, Schaffhauserstrasse 24, 8006 Zurich, Switzerland; Telephone: (00411) 363 69 19; Contact person: Dr. R.J. Hopkirk.

2.7 Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Interfacial area per unit rock volume ([m^2/m^3])</td>
</tr>
<tr>
<td>(C_k')</td>
<td>Concentration on solid of nuclide (k) (-) ([\text{atoms/m}^3 \text{ solid}])</td>
</tr>
<tr>
<td>(D_k)</td>
<td>Diffusion coefficient of nuclide (k) in fluid ([m^2/s])</td>
</tr>
<tr>
<td>(F)</td>
<td>Cross-section for flow at inlet ([m^2])</td>
</tr>
<tr>
<td>(k)</td>
<td>Nuclide index</td>
</tr>
<tr>
<td>(K_m)</td>
<td>Mass transfer coefficient ([m^3/m^2])</td>
</tr>
<tr>
<td>(N_k)</td>
<td>Concentration in water of nuclide (k) ([\text{atoms/kg water}])</td>
</tr>
<tr>
<td>(R_k)</td>
<td>Retention factor for nuclide (k) ([\text{-}])</td>
</tr>
<tr>
<td>(T)</td>
<td>Leaching duration ([s])</td>
</tr>
<tr>
<td>(t)</td>
<td>Time ([s])</td>
</tr>
<tr>
<td>(V)</td>
<td>Water velocity ([m/s])</td>
</tr>
<tr>
<td>(x)</td>
<td>Space coordinate ([m])</td>
</tr>
<tr>
<td>(\varepsilon)</td>
<td>Effective porosity ([\text{-}])</td>
</tr>
<tr>
<td>(\lambda_k)</td>
<td>Decay constant of nuclide (k) ([s^{-1}])</td>
</tr>
<tr>
<td>(\rho)</td>
<td>Water density ([\text{kg/m}^3])</td>
</tr>
</tbody>
</table>

Zurich, 18th May 1983
1. MODEL CHARACTERIZATION

1.1 Equations

\[ \frac{R_i^f}{\partial t} \frac{\partial S_i}{\partial t} + V \frac{\partial S_i}{\partial z} + R_i^f \lambda_i S_i = 0 ; \]

\[ R_i^f \frac{\partial S_i}{\partial t} + V \frac{\partial S_i}{\partial z} + R_i^f \lambda_i S_i - R_i^f \lambda_{i-1} S_{i-1} = 0 ; i = 2, 3 \]

1.2 Basic Assumptions:

(a) one-dimensional transport
   homogeneous medium
   instantaneous linear sorption equilibrium

(b) arbitrary time dependent plane source.

1.3 Initial Conditions

\[ S_i(z, t) = 0 \quad \text{at} \ t = 0 \]

1.4 Boundary Conditions

1.4.1 Flow

\[ S_i(z, t) \text{ at } z = 0 \text{ equals the geosphere input of radionuclide } i \text{ at time } t. \]

As \( z \) and \( t \) approach infinity \( S_i(z,t) \) remains finite.
1.4.2 Equations 1.1 are solved for a delta function flux boundary condition at \( z = 0 \). The resulting response functions, given in Table 1 attached, are convoluted with the geosphere input.

1.5 Restriction on Parameters:

\[
R_i^f \neq R_j^f, \text{ for } K \neq K
\]

1.6 References:


2. CODE CHARACTERIZATION

2.1 Name of Code

GARD2S - Geochemical Assessment of Radionuclide Disposal (A SYVAC implementation).

2.2 Method of Solution

Analytical solutions based on Laplace Transforms.

2.3 Restriction in Parameter Values

-

2.4 Size of Code and Programming Language

FORTRAN IV.

The convolution routine is part of the larger SYVAC code and totals about 3000 statements.

2.5 Application of Code

Atomic Energy of Canada Limited

Environmental and safety assessment of permanent disposal of un-reprocessed spent nuclear fuel in a waste vault located in a pluton on the Canadian Shield.
2.6 Availability

Environmental and Safety Assessment Branch
Whiteshell Nuclear Research Establishment
Pinawa, Manitoba, Canada.

NOMENCLATURE

\( R_f^i \) = surface based retention factor for nuclide \( i \)
\( R_f^i = 1 + Ka/b \)

\( 2b \) = crack width (m) ; \( Ka \) = Surface based distribution coefficient (m\(^2\))

\( S_i \) = flow rate of radionuclide \( i \) in groundwater at position \( z \) and at time \( t \) (mol/a)

\( V \) = groundwater velocity (m/a)

\( z \) = distance from vault along one-dimensional flow path (m)

\( t \) = time from the sealing of the vault (a)

\( \lambda_i \) = decay constant of radionuclide \( i \) (a\(^{-1}\))
GEOSPHERE RESPONSE FUNCTIONS FOR THE GEOSPHERE
FOR A THREE-MEMBER DECAY CHAIN*

\[
R_{ij}^k = \exp (-\omega K_j) \delta(t-t' - \omega K_j) \quad \text{where} \quad i=1,2,3, \quad j=1
\]

\[
R_{ij}^k = \frac{K_j}{K_i - K_j} \exp \left\{ \frac{K_j}{K_i - K_j} (t-t' - K_i \omega - K_j \omega) \right\}
\]

\[
\cdot (h(t-t' - K_i \omega) - h(t-t' - K_j \omega)) \quad \text{where} \quad i=1,2, \quad j=i+1
\]

\[
R_{ij}^k R_{ij}^l = \frac{K_j \lambda_i K_{ij}^2}{(K_j - K_i) (K_j - K_{ij}) - (K_j - K_i) (K_j - K_{ij})}
\]

\[
\exp \left\{ \frac{K_j \lambda_i (t-t' - K_i \omega - K_j \omega)}{K_i - K_j} \right\}
\]

\[
\cdot (h(t-t' - K_i \omega) - h(t-t' - K_j \omega))
\]

\[
\frac{K_j \lambda_i (t-t' - K_i \omega) - K_j \lambda_i (t-t' - K_i \omega)}{K_i - K_j}
\]

\[
\cdot (h(t-t' - K_i \omega) - h(t-t' - K_j \omega))
\]

where,

\( R_{ij}^k \) is the geosphere response function for input of nuclide \( i \) resulting in output of nuclide \( j \)

\( \omega \) is the groundwater transit time = transit length x travel time

\( \delta(t) \) is the Dirac delta function

\( h(t) \) is the Heaviside step function

\( \lambda_i \) is radioactive decay constant of nuclide \( i \) (s\(^{-1}\))

\( K_i \) is the retardation factor of nuclide \( i \) in geosphere

\( t \) is the time of output

\( t' \) is the time of input

* Radionuclide 1 decays to radionuclide 2, which in turn, decays to radionuclide 3, which is also radioactive.
1. Model Characterization

1.1 Governing Equations

Ground Water Flow

The differential equation describing the steady-state hydraulic head distribution in a nonhomogeneous anisotropic flow regime where the principal components of the hydraulic conductivity tensor are coincident with the coordinate axes can be written in two dimensions as

\[ L(h) = \frac{\partial}{\partial x} (K_{xx} \frac{\partial h}{\partial x}) + \frac{\partial}{\partial z} (K_{zz} \frac{\partial h}{\partial z}) = 0 \]

where \( L \) is the differential operator defined in the flow regime, \( h \) is the hydraulic head, \( x \) and \( z \) are the Cartesian directions and \( K_{xx} \) and \( K_{zz} \) are the principal components of the hydraulic conductivity tensor. It is assumed that \( K_{xx} \) and \( K_{zz} \) can vary spatially but are constant within each element.

The Darcy velocities can be expressed as

\[ q_x = -K_{xx} \frac{\partial h}{\partial x} \]
\[ q_z = -K_{zz} \frac{\partial h}{\partial z} \]

where \( q_x \) and \( q_z \) are the Darcy velocities in the \( x \) and \( z \) directions respectively. The average interstitial porewater velocities are calculated by dividing the Darcy velocities by the porosity. This is expressed
APPENDIX 2:67

\[ V_x = \frac{q_x}{\theta} \]
\[ V_z = \frac{q_z}{\theta} \]

where \( V_x \) and \( V_z \) are the average interstitial porewater velocities and \( \theta \) is the porosity. It is assumed that \( \theta \) can vary spatially but is a constant within each element.

**Solute Transport**

A general equation describing solute transport in a saturated porous medium can be written in two dimensions as

\[
(\theta + \rho K_d) \frac{\partial C}{\partial t} = \frac{\partial}{\partial x}(\theta D_{xx} \frac{\partial C}{\partial x} + \theta D_{xz} \frac{\partial C}{\partial z} - q_x \frac{\partial C}{\partial x}) \\
+ \frac{\partial}{\partial z}(\theta D_{zx} \frac{\partial C}{\partial x} + \theta D_{zz} \frac{\partial C}{\partial z} - q_z \frac{\partial C}{\partial z}) - \lambda(\theta + \rho K_d)C
\]

where \( \theta \) is the porosity of the medium, \( \rho \) is the bulk density of the medium, \( K_d \) is the distribution coefficient relating the concentration of solute in the sorbed and solution phases, \( C \) is the concentration of the constituent in solution, \( t \) is time, \( x \) and \( z \) are the Cartesian coordinate directions, \( D_{xx} \), \( D_{xz} \), \( D_{zx} \), and \( D_{zz} \) are the hydrodynamic dispersion coefficients, \( q_x \) and \( q_z \) are the Darcy velocities in the \( x \) and \( z \) directions, respectively and \( \lambda \) is a first-order reaction constant (e.g. radioactive decay).

The components of the hydrodynamic dispersion tensor include the effects of mechanical dispersion and molecular diffusion and are written

\[
\theta D_{xx} = \frac{\alpha_L q_x^2}{q} + \frac{\alpha_T q_z^2}{q} + \theta D^* 
\]
\[ \theta D_{zz} = \frac{a_T q_x^2}{\bar{q}} + \frac{a_L q_z^2}{\bar{q}} + \theta D^* \]

\[ \theta D_{xz} = \theta D_{zx} = \frac{(a_L - a_T) q_x q_z}{\bar{q}} \]

where \( a_L \) and \( a_T \) are the longitudinal and transverse dispersivities, respectively of the medium, \( \bar{q} \) is the resultant Darcy velocity and \( D^* \) is the diffusion coefficient of the solute in the porous medium.

1.2 Basic Assumptions

- Two-dimensional ground-water flow and solute transport;
- Fluid flow may be described by Darcy's law;
- Steady-state ground water flow;
- Solute transport equation includes advection, dispersion, diffusion, adsorption (linear reversible) and first-order reactions such as radioactive decay;
- System properties may vary spatially.

1.3 Initial Conditions

The initial conditions necessary for the solution of the solute transport equation are

\[ C(x,z,0) = \tilde{C}_o(x,z) \]

where \( \tilde{C}_o \) are prescribed concentrations.
1.4 Boundary Conditions

The boundary conditions for the ground water flow equation can be Dirichlet expressed as

\[ h(x,z) = h(x,z) \quad \text{on } \Gamma_1 \]

and Neumann expressed as

\[ (K_{xx} \frac{\partial h}{\partial x} + K_{zz} \frac{\partial h}{\partial z}) \cdot \mathbf{n} = - q_n^h \quad \text{on } \Gamma_2 \]

where \( \Gamma_1 + \Gamma_2 = \Gamma \), the total boundary of the system, \( h \) are prescribed hydraulic heads and \( q_n^h \) is the prescribed liquid flux across a Neumann boundary and \( \mathbf{n} \) is the unit outward normal vector to the boundary.

The boundary conditions for the solute transport equation can be Dirichlet expressed as

\[ C(x,z,t) = C(x,z,t) \quad \text{on } \Gamma_1 \]

Neumann expressed as

\[ (\Theta_{xx} \frac{\partial C}{\partial x} + \Theta_{xz} \frac{\partial C}{\partial z} + \Theta_{xx} \frac{\partial C}{\partial x} + \Theta_{zz} \frac{\partial C}{\partial z} \cdot \mathbf{n} = 0 \quad \text{on } \Gamma_2 \]

and Cauchy, or mixed, expressed as

\[ (\Theta_{xx} \frac{\partial C}{\partial x} + \Theta_{xz} \frac{\partial C}{\partial z} + \Theta_{xx} \frac{\partial C}{\partial x} + \Theta_{zz} \frac{\partial C}{\partial z} + q_x C + q_z C) \cdot \mathbf{n} = (q_x \hat{C} + q_z \hat{C}) \cdot \mathbf{n}, \quad \text{on } \Gamma_3 \]

where \( \Gamma_1 + \Gamma_2 + \Gamma_3 = \Gamma \), the total boundary of the system, \( \mathbf{n} \) is the outward normal vector to the boundaries \( \Gamma_2 \) and \( \Gamma_3 \), and \( \hat{C} \) are prescribed concentrations of the solute at a solute influx boundary.
1.5 **Restriction in Parameters**

----------

1.6 **References**


2. **Code Characterization**

2.1 **Name of code**

TRANSAT: Solute Transport in Saturated Geologic Media

2.2 **Method of Solution**

Numerical solution - finite element method
- utilizes linear triangular elements spatially
- utilizes backward difference in time
- gaussian elimination solver
2.3 Restriction in Parameter Values

Suggested:

Courant Number

\[ C_0 = \frac{V \Delta t}{\Delta x} < 1 \text{ at early time} \]

Mesh Peclet

\[ Pe = \frac{V \Delta x}{D} < 1 \]

2.4 Size of Code and Programming Language

1400 program statements
Fortran IV

2.5 Applications of the Code

- Analysis of field tracer test data for the determination of transport parameters;
- Analysis of laboratory tracer data for investigation of solute transport in fractured/porous media;
- Simulation of groundwater flow from waste lagoons;
- Simulation of radionuclide transport in geologic media;
- Seepage analysis of groundwater flow into a proposed open-pit uranium mine;
- Assessment of contaminant transport from an organic toxic waste disposal site;
2.6 Availability

GTC Geologic Testing Consultants Ltd.
785 Carling Avenue, 4th Floor
Ottawa, Ontario
Canada K1S 5H4

Telephone: (613) 563-4331 Telex: 053-4307

Nomenclature

- Identified in Governing Equations (Section 1.1)
1.0 MODEL CHARACTERIZATION

1.1 Transport Equations

\[ \frac{\partial M_k(x,t)}{\partial t} = - \frac{\partial V M_k(x,t)}{\partial x} + D \frac{\partial^2 M_k(x,t)}{\partial x^2} \]

\[ - \lambda_k M_k(x,t) + \lambda_{k-1} M_{k-1}(x,t) - \frac{c}{\rho} U_k(x,t) \]

\[ \frac{\partial S_k(x,t)}{\partial t} = - \lambda_k S_k(x,t) + \lambda_{k-1} S_{k-1}(x,t) + U_k(x,t) \]

where \( U_k(x,t) \) is defined as:

\[ U_k(x,t) = \frac{K \lambda_k M_k(x,t)}{\partial t} \]

or

\[ U_k(x,t) = \frac{\rho c \lambda_k M_k(x,t) - \lambda_{k-1} S_{k-1}(x,t)}{\partial t} \]

or

\[ U_k(x,t) = nK \frac{\partial M_k(x,t)^{n-1}}{\partial t} \]

or others.

1.2 Basic Assumptions

1. one-dimensional transport

2. homogeneous medium

3. dilute solution, that is the water flow is not affected by nuclides, and nuclides do not affect the chemistry of each other except through radioactive decay

4. arbitrarily time dependent plane source.
1.3 Initial Conditions

\[ M_k(x,0) = 0 \]

1.4 Boundary Conditions

1.4.1 Upstream

1. \( M_k(0,t) \) arbitrary time dependent concentration at inlet

or

2. \( J_k(0,t) \) arbitrary time dependent flux at inlet

2. \( \frac{\partial M_k(0,t)}{\partial x} = 0 \) reflection boundary condition

1.4.2 Downstream

a) \( M_k(x^+,t) = 0 \) concentration boundary at \( x > x_0 \), that is

a no return or infinite dilution boundary condition with discontinous concentration at the boundary.

1.5 Restriction in Parameters

None.

1.6 References

2.0 CODE CHARACTERIZATION

2.1 Name of Code

DRAMA

2.2 Method of Solution

A direct simulation that uses a large number of discrete particles to carry the nuclides. Dispersion is handled by a random walk technique.

2.3 Restrictions in Parameter Values

None, except that large retention factors and/or large dispersion coefficients require large amounts of computer time (measured in hours).

2.4 Size of Code and Programming Language

The program has 3200 lines, of which 1400 are comments. The program is written in FORTRAN IV, with dynamic memory management.

2.5 Applications of the Code

Comparing different chemical models such as the \( K_d \) model and the Freundlich isotherm.

2.6 Availability

The program could be made available, but at present there is very little documentation for it.
NOMENCLATURE

The following variables are used in addition to the nomenclature supplied by INTRACOIN.

1. $J_k$ flux of nuclide $k$ [Moles/(m$^2$t)]

2. $K$ constant in Freundlich isotherm

3. $k_1$ rate constant for kinetic chemistry [1/t]

4. $k_2$ rate constant for kinetic chemistry [1/t]

5. $n$ power exponent in Freundlich isotherm

6. $M_k$ concentration in water of nuclide $k$ [Moles/m$^3$ water]

7. $S_k$ concentration on solid of nuclide $k$ [Moles/ks solid]

8. $v$ advective water velocity [m/t]

9. $x_0$ location of downstream (exit) boundary

10. $x_0^*$ location outside downstream boundary
APPENDIX 2:77

MODEL AND CODE CHARACTERIZATION: COLUMN

Project team: KEMAKTA Consultants Co, Stockholm, SWEDEN.

1. Model Characterization

1.1 Transport Equation

\[
\frac{dC_k}{dt} = \frac{D}{r} \frac{\partial^2 C_k}{\partial x^2} - \frac{V}{R_k^p} \frac{\partial C_k}{\partial x} + \lambda_{k-1} C_{k-1} - \lambda_k C_k
\]

Where the derivative on the left is the concentration in a local liquid volume that follows the movement (V/R^p_k) of the component k in the liquid phase.

1.2 Assumptions

a. One dimensional transport.

b. Piecewise homogenous media or continuously varying material properties.

c. Arbitrarily time- and, or space dependent retention.

d. Arbitrarily time dependent plane source

1.3 Initial conditions

C_k(x,0) = 0

1.4 Boundary conditions

1.4.1 Upstream

1. C_k(x,t) for x < 0 Arbitrary time dependent concentration at inlet.

2. R_k^p(x,t) for x < 0 Arbitrary retention factors at inlet

1.4.2 Downstream

1. C_k(x=0,t) = 0 (Semi-infinite medium)

2. \[ \frac{\partial C_k}{\partial x} = 0 \] for x = L

1.5 Restrictions in parameters

Only those dictated by numerical problems.
2 Code characterization

2.1 Name_of_code

Column

2.2 Method_of_solution

Numerical

Method of characteristics

1 Moving grid. The grid points move \( V/R_k \) times the time increment for each time step.

2 The concentrations in the new grid points are calculated before integration by cubic spline interpolation in the previous grid.

3 Integration is performed on the moving grid.

The finite difference approximations used for the integration in space are:

\[
\frac{\partial C_k}{\partial x} = \frac{1}{2} \left( \frac{C_{k+1}^L - C_k^L}{h_{L+}} + \frac{C_k^L - C_{k-1}^L}{h_{L-}} \right)
\]

\[
\frac{2C_k}{x^2} = \frac{2}{h_{L+} h_{L-}} \left( \frac{C_{k+1}^L - C_k^L}{h_{L+}} - \frac{C_k^L - C_{k-1}^L}{h_{L-}} \right)
\]

For the integration in time the forward difference

\[
\frac{dC_k}{dt} = \frac{C_k(L,n+1) - C_k(L,n)}{j}
\]

is used

where \( n \) enumerates time and \( j \) is the time increment.
2.3 Restrictions in parameter values
\[ 0.5r_D \frac{K}{D} (\text{space step})^2 \]
Time step \( \ll \)

Cautious choice of retention values has to be made for \( x < 0 \) and \( x > L \) so as not to cause a severe depletion of grid points covering the region of interest.

2.4 Size of code and programming language
Approximately 300 statement lines in FORTRAN IV

2.5 Computer requirements
2.5.1 Computer
Amdahl 470 OS:VS2/MVS-JES2
2.5.2 Time for one multiplication
3.0E-7 s.
2.5.3 Requirements for INTRACOIN Case 1 (T2,L1,I2,R1,P2)
Time 39.3 s.
Storage 184 K bytes
APPENDIX 2:80

CODE: PORFLO

PROJECT TEAM: GeoTrans, Inc.

1.0 MODEL CHARACTERIZATION

PORFLO is a finite difference code designed to simulate time-dependent or quasi-steady-state processes consisting of coupled ground-water flow, heat transfer, and transport of a single radionuclide species in a porous medium. The code is applicable to problems in two dimensions over a rectangular or axially symmetric cylindrical domain.

1.1 TRANSPORT EQUATION

The mathematical model in PORFLO is based on the physical laws of mass, momentum and energy conservation. The flow field is described by the governing equation for water flow. The temperature distribution is described by the energy balance equation. The radionuclide migration is described by the advective-dispersive solution transport equation. Discussion on the theoretical basis can be found in Baca et al. (1912, 1983) and in the site characterization report by Rockwell (1982).

The solute transport equation considered in the PORFLO code takes the form

\[
\frac{\partial R_d \frac{\partial c}{\partial t}}{\partial x} + U \frac{\partial c}{\partial x} + V \frac{\partial c}{\partial y} = \frac{\partial}{\partial x} \left( D_{xx} \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial y} \left( D_{yy} \frac{\partial c}{\partial y} \right) \\
- \lambda \phi R_d c + \dot{m}
\]
APPENDIX 2

Where

\[ R_d = \text{retardation factor} \]
\[ c = \text{solute concentration} \]
\[ x, y, t = \text{coordinates and time} \]
\[ U, V = \text{x and y components of Darcy velocity} \]
\[ D_{xx}, D_{yy} = \text{components of hydrodynamic dispersion tensor} \]
\[ \phi = \text{porosity of the porous medium} \]
\[ \lambda = \text{radioactive decay constant} \]
\[ \dot{m} = \text{internal mass source term, which can be time dependent} \]

1.2 BASIC ASSUMPTIONS

- Transport of the considered radionuclide component is independent from the other components. (i.e., chain reaction effects can be neglected).
- Cross component, \( D_{xy} \), of the hydrodynamic dispersion tensor can be neglected.
- Transport is governed by the combined effect of advection and hydrodynamic dispersion. The code cannot handle the case of pure advection or infinite \( Re \) or \( Te \) number.
- Porous medium is unfractured.

1.3 INITIAL CONDITION

\[ c(x, y, t = 0) = c^0 \]

1.4 BOUNDARY CONDITIONS

PORFLO can handle both prescribed concentration and prescribed flux boundary conditions. However, it assumes that through the period of simulation, the boundary conditions do not vary with time. Because of
this assumption, it is necessary to adopt the following procedures to solve INTRACOIN's problems: (1) run the code by regarding the radionuclide species as a conservative species with $\lambda = 0$, and (2) modify the computed concentration by a factor of $e^{\lambda t}$, where $\lambda$ is the half-life of the component considered.

1.5 RESTRICTION IN PARAMETERS

There are certain combinations of dispersivity value travel time that make the numerical simulation by PORFLO either extremely costly or impractical. Because PORFLO employs finite difference approximations (see Gosman et al., 1969) it is necessary to select the grid spacing such that $\varepsilon x/\alpha \leq 2$, where $\alpha$ is the dispersivity, to avoid numerical difficulties. If the dispersivity is small and the groundwater velocity is large, the code may require excessive number of nodes and time steps.

1.6 REFERENCES


APPENDIX 2:83


2.0 CODE CHARACTERIZATION

2.1 Name of Code - PORFLO

2.2 Method of Solution

Finite difference approximation

2.3 Restriction in parameter values

Pe must not be excessively large.

Need to control the grid such that $\Delta x/a<2$.

Need to control the time step such that $V\Delta t/\Delta x<1$.

2.4 Sign and Language

3,500 lines of FORTRAN IV

2.5 Applications

APPENDIX 2:84


2.6 Availability

Available through Rockwell International, Basalt Waste Isolation Project.
1.0 MODEL CHARACTERIZATION

1.1 Transport Equation

The flow field is approximated by a network of "pipes" corresponding to the stream tube segments. Within each pipe, if nuclide $k$ is not formed by radioactive decay, the concentration is

$$
\frac{\partial c_k}{\partial t} + v \frac{\partial c_k}{\partial x} = \frac{a_L}{R_k} \frac{\partial^2 c_k}{\partial x^2}
$$

where

$$
c_k = \frac{c_k e^{-\lambda_k t}}{I_k}
$$

If nuclide $k$ is formed by decay of nuclide $k'$, then the concentration is given by

$$
c_k = c_k' I_k(t) \frac{R_k'}{R_k}
$$

where $I_k(t)$ is the total inventory of nuclide $k$, found by solving the Bateman equation for the entire decay chain. More complex versions of this last formula are used in certain circumstances.

1.2 Basic Assumptions

- The flow field can be divided into stream tubes, not excessively curved, within which the flow is fairly homogeneous.
- Half lives of daughter nuclides are small compared to both the time required for the pulse of parent to traverse the outlet, and the time required for the daughter to traverse the final pipe. (This assumption can be relaxed in some circumstances.)
• Peclet number large enough for concentration and input boundary conditions to be roughly equivalent. (Importance of this assumption is unclear.)

• Flow field is piecewise constant, with only "jump" changes.

• Transverse dispersion can be neglected, except in a two-dimensional aquifer with uniform velocity.

1.3 Initial Conditions

\[ c = 0 \]

1.4 Boundary Conditions

Each pipe has a prescribed input. However, the Green's function used to calculate transport within a pipe is derived by assuming B.C.'s of \( c = 0 \) at \( \pm \infty \).

1.5 Restriction in Parameters

There are certain combinations of half-lives and travel times which make the formula for daughter nuclide releases represent only an upper bound. The formulae are complex and are found in the user's guide.

1.6 References


2.0 CODE CHARACTERIZATION

2.1 Name of Code - NUTRAN

2.2 Method of Solution

Green's function within each segment in a network of "pipes".

2.3 Restriction in Parameter Values

Pe < 1.5 within any pipe makes the assumptions regarding B.C.'s incompatible.

2.4 Size and Language

7000 lines of PL/1

2.5 Applications


Study of hypothetical salt repositories using sensitivity and uncertainty analysis techniques.

Forthcoming NUREG/CR.

Analysis of engineered barrier performance in a repository.

2.6 Availability

Available shortly through Argonne Code Center. (Currently undergoing acceptance testing.)
NWFT/DVM
GENERALIZED NETWORK

1. Model Characterization

NWFT/DVM models fluid flow and the transport of radionuclide chains in a porous medium. Flow fields are represented as a network of one-dimensional path segments or "legs". A steady-state water velocity is calculated in each leg, with pressures and brine densities considered. The release of radionuclides to ground water is determined by the combined effects of kinetic leaching and equilibrium solubility. Transport of radionuclides can be handled by either an analytic solution or by the Distributed Velocity Method (DVM) which is unique to this code.

1.1 Equations

Fluid flow is calculated by simultaneously solving, for all legs, the following equations:

\[ q_{ij} = \frac{1}{R_{ij}} \left( P_i - P_j \right) + \rho_{ij} \left( D_i - D_j \right) \]  

(1)

and

\[ \sum_{i \neq j} q_{ij} = 0 \]  

(2)

where \( q_{ij} \) is the flow along the path from node i to node j, \( P \) and \( D \) are the pressure and elevation at each node, respectively, \( \rho_{ij} \) is the average fluid density in the leg, and \( R_{ij} \) is a "hydraulic resistance" defined by

\[ R = \frac{\mu L}{k A} \]  

(3)

where \( \mu \) is the viscosity of the fluid in the leg, \( L \) is the leg length, \( k \) is the permeability, and \( A \) is the cross-sectional area. Water density and viscosity are functions of brine density.

Transport can be handled in two ways: analytically or by the DVM method. Analytical transport is limited to chains of three or fewer nuclides having the same retardation factor. Solubility limits are not considered and the equations used are:
\[
N_1(t) = \frac{N_1(0)}{2\tau} e^{-\lambda_1 t} [U(t) - U(t-\tau)H(t-\tau)] \\
\]

\[
N_2(t) = \left[ \frac{N_2(0)}{2\tau} e^{-\lambda_2 t} + \frac{N_1(0)}{2\tau} \left( \frac{\lambda_1}{\lambda_2 - \lambda_1} \left( e^{-\lambda_1 t} - e^{-\lambda_2 t} \right) \right) \right] \\
[U(t) - U(t-\tau)H(t-\tau)] \\
\]

\[
N_3(t) = \left[ \frac{N_3(0)}{2\tau} e^{-\lambda_3 t} + \frac{N_2(0)}{2\tau} \left( \frac{\lambda_2}{\lambda_3 - \lambda_2} \left( e^{-\lambda_2 t} - e^{-\lambda_3 t} \right) \right) + \right. \\
\left. \frac{N_1(0)}{2\tau} \frac{\lambda_1 \lambda_2}{(\lambda_2 - \lambda_1) (\lambda_3 - \lambda_2)} \left( e^{-\lambda_1 t} - e^{-\lambda_2 t} \right) + \frac{e^{-\lambda_2 t}}{(\lambda_1 - \lambda_2) (\lambda_3 - \lambda_2)} \right] \\
[U(t) - U(t-\tau)H(t-\tau)] \\
\]

where

\[ t = \text{time (days)} \]
\[ N_1(0) = \text{inventory of isotope i at time } t = 0 \text{ (Ci)} \]
\[ \lambda_i = \text{decay constant of isotope i (days)} \]
\[ \tau = \text{leach time (days)} \]
\[ H(x) = 0 \quad x < 0 \]
\[ H(x) = 1 \quad x \geq 0 \]

and the function \( U(t) \) is given by

\[
U(t) = \text{erfc} \left( \frac{L_p - \tilde{\nu} t}{\sqrt{4\alpha \tilde{v} t}} \right) + e^{\frac{L_p}{\alpha}} \text{erfc} \left( \frac{L_p + \tilde{\nu} t}{\sqrt{4\alpha \tilde{v} t}} \right) \\
\]

where

\[ \alpha = \text{dispersivity (ft)} \]
\[ \frac{\tilde{\nu}}{\nu} = \text{average isotope velocity accounting for retardation (ft/day)} \]
\[ L_p = \text{distance from source to discharge point (ft)} \]
\[ \text{erfc} = \text{complementary error function}. \]
The distributed velocity method (DVM) is based on dividing the path into cells. Dispersion is treated by dividing the contaminant in each cell into pockets with different velocities. The velocities, of which there are N, are chosen so as to divide a Gaussian distribution of velocities into intervals of equal area. For a single species, the amount \((i,t)\) of the species arriving in cell \(i\) at time step \(t\) is given by

\[
p(i,t) = \frac{D}{N} \sum_j M_j \rho(i-k_j,t-1) \\
+ (1-M_j) \rho(i-k_j-1,t-1)
\]

(8)

In this equation, \(D\) represents radioactive decay:

\[
D = e^{-\lambda \Delta t}
\]

(9)

where \(\lambda\) is the decay constant and \(\Delta t\) is the time step; \(k_j\) is the number of entire cells that can be traversed in one time step at velocity \(V_j\):

\[
k_j = \left\lfloor \frac{V_j \Delta t}{\Delta x} \right\rfloor
\]

(10)

The double bars indicate the integral part.

\(M_j\) is the fraction of cell \(i-k_j\) which lies a distance \(V_j \Delta t\) from points within cell \(i\):

\[
M_j = k_j + 1 - \frac{V_j \Delta t}{\Delta x}
\]

(11)

1.2 Basic Assumptions

One-dimensional steady-state laminar flow; one-dimensional solute transport equation is valid within each path segment; brine concentrations and pressures are constant over time; sorption can be represented as equilibrium adsorption; pathway dimensions, permeability, porosity, and brine density are averaged along each path segment.

1.3 Boundary Conditions

Pressures at the inlet and outlet nodes of the flow system network.
APPENDIX 2:91

1.4 Restriction in Parameters

None

1.5 References


"NWFT/DVM Lecture Notes" (rough draft), Sandia National Laboratories.

Campbell, J. E., D. E., Longsine, and M. Reeves, "The Distributed Velocity Method of Solving the Convective-Dispersion Equation," to be published.

2. Code Characterization

2.1 Name of Code

NWFT/DVM: Network Flow and Transport/Distributive Velocity Method

2.2 Method of Solution

Semi-Analytical

2.3 Restriction in Parameter Values

To avoid numerical dispersion, the most important parameter to consider is the Courant number, C, defined by

\[ C(r) = \frac{v(r) \Delta t}{\Delta x} \]

where \( r \) is the isotope, \( \bar{v} \) is the mean velocity of isotope \( r \), \( \Delta t \) is the time step, and \( \Delta x \) is the grid block size. For DVM, \( C \geq 1 \) and must be adjusted so that each isotope, if possible, satisfies this criterion. Hence, it is advantageous to maximize the time step and minimize the grid block size to decrease numerical dispersion.

2.4 Size of Code and Programming Language

4000 program statements; CDC FORTRAN IV.
2.5 Application of Code

NWFT/DVM is a far-field code. The generalized network allows for the modeling of detailed sedimentary stratigraphy. One of its greatest strengths is in handling situations involving (1) decay chains with moderate contrasts in half-life and retardation factors, which cause difficulties for analytic and Green's function codes, and (2) path lengths much greater than the dispersivity, which are difficult to analyze with finite-element and finite-difference methods.

2.6 Availability

Sandia National Laboratories (Albuquerque, New Mexico) and the NRC (Nuclear Regulatory Commission).
SWIFT II is a fully transient, three-dimensional model which simulates the flow and transport of fluid, heat (energy), brine and radionuclide chains in porous and fractured geologic media. The primary equations for fluid, heat and brine are coupled by fluid density, fluid viscosity and porosity. Steady-state options are available for the fluid and brine equations and both Cartesian and cylindrical coordinate systems may be used. (The latter system is restricted, however, to two-dimensional r-z simulations). Both dual-porosity and discrete-fracture conceptualizations may be considered for the fractured zone. Migration within the rock matrix is characterized as a one-dimensional process. A comprehensive discussion of the model is given by Reeves, Johns and Crarwell [1984a].

2.1 EQUATIONS

SWIFT II comprises the four transport processes: fluid, heat, brine and radionuclide chains. For a porous media only the global (three-dimensional) process simulator is used. For a fractured media the global process simulator is used for the fractured media, and the local (one-dimensional) process simulator is used for the rock matrix. In the INTRACOIN Level-1 calculations, only the steady-state fluid and transient-state radionuclide transport equations were invoked. For these cases, the equations specialize to:

**Fluid (Global):**

\[- \nabla (\rho u) - q - q_w = 0\]

conduction production sink/source
APPENDIX 2:94

Radionuclide r (Global):

\[- \nabla \cdot (\rho_C \vec{u}) + \nabla \cdot (\rho_E \nabla \varepsilon r) = C_r \dot{q}_r - q_r + q_{wr}\]

- \(\dot{q}_r\): convection
- \(\nabla \cdot (\rho_E \nabla \varepsilon r)\): dispersion/
diffusion
- \(C_r\): produced component
- \(q_r\): sink/source
- \(q_{wr}\): waste

\[- \Gamma_r + \sum_{s=1}^{N} k_{rs} \lambda_s [\phi \rho_s + (1-\phi) \rho_r \dot{w}_s]\]

- \(\Gamma_r\): loss to matrix
- \(k_{rs}\): generation of component
- \(\lambda_s\): r by decay of s

- \(\lambda_r [\phi \rho_C + (1-\phi) \rho_r \dot{w}_r] = \frac{3}{\partial t} [\phi \rho_C + (1-\phi) \rho_r \dot{w}_r]\)

- \(\partial_t\): decay of component r
- \(\dot{w}_r\): accumulation

Radionuclide r (Local):

\[- \nabla \cdot (\rho'C' \vec{u}') + \nabla \cdot (\rho'E' \nabla \varepsilon r') = \sum_{s=1}^{N} k_{rs} \lambda_s k_s \phi \rho_s \varepsilon s\]

- \(\nabla \cdot (\rho'E' \nabla \varepsilon r')\): generation of component
- \(\varepsilon_s\): r by decay of s

\[- \lambda_0 k_0 \phi \rho'C' + (\varepsilon_{r'} + \Gamma_{r'}) = \frac{3}{\partial t} (k_0 \phi \rho'C')\]

- \(\partial_t\): decay of component r
- \(\Gamma_{r'}\): gain from fracture
- \(\varepsilon_{r'}\): accumulation

where:

- \(C\): radionuclide mass fraction
- \(E_C\): dispersion tensor, which is related to the longitudinal and transverse dispersivitivities and the molecular diffusivity in a conventional manner
- \(k_{rs}\): radionuclide branching ratio
- \(K_r\): retardation factor
- \(q\): fluid discharge
- \(u\): Darcy velocity vector
APPENDIX 2:95

\[ W_r \] = solid-phase concentration, which is related to the liquid-phase concentration by a Freundlich isotherm

\[ \Gamma_r \] = radionuclide transfer from fracture to matrix

\[ \lambda \] = radionuclide decay constant

\[ \phi \] = porosity

\[ \rho \] = fluid density

\[ \rho_R \] = rock density

A prime indicates a property of the local rock-matrix subsystem.

2.2 BASIC ASSUMPTIONS AND CHARACTERISTICS

- Three-dimensional transport in the global system and one-dimensional transport in the local rock-matrix subsystem.
- Local rock matrix may be characterized by either prisms or spheres.
- Single-phase fluid flow governed by Darcy's Law.
- Linear variations in porosity and fluid density with respect to the dependent variables.
- Viscosity is dependent on temperature and brine concentration only.
- Non-linear isothermal equilibrium adsorption (Freundlich or linear).
- Confined or unconfined aquifer (A transient or steady-state free-water surface is available for the later)
- Hydraulic and thermal conductivities may be heterogeneous and/or anisotropic.
- Longitudinal and transverse dispersivities may vary throughout the domain.
- Molecular diffusion is constant in the global system. (A temperature dependence is permitted in the local rock-matrix subsystem).
- Other properties such as heat capacity and salt-dissolution constants may vary throughout the domain.
2.3 BOUNDARY CONDITIONS

For INTRACOIN Level-1 Problems the one and two-dimensional velocity fields were simulated with constant-pressure (Dirichlet) boundary conditions and with wells. Radionuclides were then introduced through a waste-leach submodel by means of which prescribed inventories were released at a constant rate of a given time of leach. Other boundary-condition options, which were not used for this problem set, include the following: Dirichlet fixed conditions for brine concentrations and temperatures; radiation; fluid, brine and energy injection/withdrawals through wells; and several aquifer-influence functions deriving from an aquifer located external to the reservoir being simulated. Initial concentrations may be prescribed on a block-by-block basis but were taken to be zero for each of the INTRACOIN Level-1 Problems. Other initial condition options, which were not used herein, include hydrostatic equilibrium for the initial pressure distribution and linear interpolation of a prescribed table of temperature versus depth.

2.4 RESTRICTION OF PARAMETERS

None.

2.5 REFERENCES


3 CODE CHARACTERIZATION

3.1 NAME OF CODE

_Sandia Waste-Isolation_ Flow and _Transport Model II (SWIFT II)._ 

3.2 METHOD OF SOLUTION

Discretization is performed by the finite-difference method using centered or backward weighting in the time and space domains. Matrix solution is performed either by Gaussian elimination or by two-line successive overrelaxation.

3.3 RESTRICTION IN PARAMETER VALUES

Conventional finite-difference numerical criteria for the space and time increments must be considered in order to achieve a stable and accurate solution.

3.4 SIZE OF CODE AND PROGRAMMING LANGUAGE

82 subroutines, over 20,000 lines, FORTRAN IV.

3.5 APPLICATIONS OF CODE

- Radioactive waste in both fractured and unfractured geologic formations.
- Well-test interpretation (flow and transport).
- Thermal energy storage in aquifer.
- Contaminant migration from landfills.
3.6 AVAILABILITY

Under review by the U.S. Nuclear Regulatory Commission, by Sandia National Laboratories and by GeoTrans, Inc. Date of availability has not been determined at the present time.
APPENDIX 2:100

CODE:DPCT
PROJECT TEAM: NRC

1. MODEL CHARACTERIZATION

1.1. Equations

Ground-water flow equation:
\[ \nabla \cdot V(x, z) = 0 \]
\[ \varepsilon V(x, z) = \overline{K} \cdot \varphi H(x, z) \]
\[ \overline{K} = \begin{bmatrix} K_x & 0 \\ 0 & K_y \end{bmatrix} \]

Transport equation:
\[ \nabla \cdot (D \cdot \nabla C_k) - \nabla \cdot (C_k V(x, z)) + S_k(x, z) = \partial \left( \varepsilon C_k R_k \right) / \partial z \]

Radioactive decay:
\[ \frac{dI_k}{dt} = -\lambda_k I_k \]

1.2. Basic Assumptions

- Ground-water flow is steady state.
- Ground-water flow field is independent of the mass distributions within the system.
- Cation exchange can be approximated as an instantaneous linear equilibrium exchange process.
- Contaminants can be represented by a relatively small number of reference particles.

1.3. Initial Conditions

\[ C_k(x, z, t = 0) = 0 \]
1.4. Boundary Conditions

Flow:
No flow \( \frac{\partial H}{\partial x} = 0 \)

Constant head \( H = \text{constant} \)

Concentration:
A) Upstream
\( C_k (-, t) = 0 \)
B) Downstream
\( C_k (+, t) = 0 \)

1.5. Restrictions in Parameters

No decay chains.

1.6. References

2. CODE CHARACTERIZATION

2.1. DPCT

2.2. Method of Solution

Hybrid Solution

2.2.1) Hydraulic head is solved for using finite elements.

2.2.2) Particle tracking method is used for transport (see equation below):

\[
\Delta x = \Delta T \left( \frac{V_x}{R_k} + \frac{V_x}{V(x, z)} \right) D_L + \frac{V_z}{V(x, z)} D_T
\]

\[
\Delta z = \Delta T \left( \frac{V_z}{R_k} + \frac{V_z}{V(x, z)} \right) D_L + \frac{V_z}{V(x, z)} D_T
\]

where:

- \( D_L = \text{RAN}_1 \left( 24 \frac{V(x, z)}{R_k} \Delta T a_L \right)^{1/2} \)
- \( D_T = \text{RAN}_2 \left( 24 \frac{V(x, z)}{R_k} \Delta T a_T \right)^{1/2} \)
- \( R_k = 1 + (\alpha f \rho_p)/(8\epsilon) \)

2.3. Restriction in Parameter Values

None.

2.4. Size of Code and Programming Language

\( \approx 1,000 \) program statements FORTRAN IV
2.5. Applications of the Code

- Examination of the consequences of disruptive features within a geologic repository.


2.6. Availability

This version of DPCT should be available at NRC in early 1984.
**Nomenclature to Model and Code Characterization**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_L$</td>
<td>longitudinal dispersion length (ft)</td>
</tr>
<tr>
<td>$a_T$</td>
<td>transverse dispersion length (ft)</td>
</tr>
<tr>
<td>$B$</td>
<td>total cation concentration in solution (mg/liter)</td>
</tr>
<tr>
<td>$C_K$</td>
<td>concentration in water for nuclide K (mg/cu.ft.)</td>
</tr>
<tr>
<td>$\mathbf{J}$</td>
<td>dispersivity tensor (ft)</td>
</tr>
<tr>
<td>$D_L$</td>
<td>longitudinal dispersion factor (ft)</td>
</tr>
<tr>
<td>$D_T$</td>
<td>transverse dispersion factor (ft)</td>
</tr>
<tr>
<td>$f$</td>
<td>selectivity coefficient for exchange (unitless)</td>
</tr>
<tr>
<td>$H$</td>
<td>hydraulic head (ft)</td>
</tr>
<tr>
<td>$I_K$</td>
<td>inventory of nuclide K (Ci)</td>
</tr>
<tr>
<td>$\mathbf{K}$</td>
<td>hydraulic conductivity tensor (ft/day)</td>
</tr>
<tr>
<td>$R_K$</td>
<td>retention factor for nuclide K (unitless)</td>
</tr>
<tr>
<td>RAN1</td>
<td>random number between -.5 and .5</td>
</tr>
<tr>
<td>RAN2</td>
<td>random number between -.5 and .5</td>
</tr>
<tr>
<td>$S_K$</td>
<td>source of nuclide K (mg)</td>
</tr>
<tr>
<td>$\Delta T$</td>
<td>size of time increment (days)</td>
</tr>
<tr>
<td>$V$</td>
<td>interstitial velocity (ft/day)</td>
</tr>
<tr>
<td>$V_X$</td>
<td>X - component of interstitial velocity (ft/day)</td>
</tr>
<tr>
<td>$V_Z$</td>
<td>Z - component of the interstitial velocity (ft/day)</td>
</tr>
<tr>
<td>$\Delta X$</td>
<td>X - coordinate displacement (ft)</td>
</tr>
<tr>
<td>$\Delta Z$</td>
<td>Z - coordinate displacement (ft)</td>
</tr>
<tr>
<td>$a$</td>
<td>cation exchange capacity (meg/gm)</td>
</tr>
<tr>
<td>$\varepsilon$</td>
<td>porosity (unitless)</td>
</tr>
<tr>
<td>$\lambda_K$</td>
<td>decay constant for nuclide K (1/day)</td>
</tr>
<tr>
<td>$p_p$</td>
<td>bulk density of the geologic media (gm/liter)</td>
</tr>
</tbody>
</table>
APPENDIX 2:105

Code: MMT1DPNL

Project Team: Pacific Northwest Laboratory (PNL), U.S. Department of Energy

1. Model Characterization
Code: MMT1DPNL

1.1 Equations

MMT1DPNL does not solve partial differential equations and utilize the typical "model-equation" approach. It is a direct simulation technique which uses a particle tracking scheme for simulating the phenomena represented by a set of partial differential equations. However, the set of partial differential equations it attempts to directly simulate are shown below. In writing these equations a trailing "a" is utilized to indicate partial differentiation with respect to parameter "a".

\[
(N_i,t) = D_i (N_i,x),x - V_i (N_i,x) - (A/HL_i) N_i + (A/HL_j) N_j
\]

where:
- \( t \) = Time (units of time).
- \( x \) = The cartesian coordinate denoting distance down the flow tube (units of length).
- \( i \) = Nuclide index (range 1-9).
- \( j \) = \( i-1 \), the parent nuclide index for daughter \( i \) and has values defined only when \( i \) is greater than 2.
- \( N_i \) = Activity concentration for nuclide \( i \) at spatial location \( x \) (units of curies/volume).
- \( D_i \) = \((d/v/ri)\), the effective dispersion constant for nuclide \( i \) (units length squared per time).

Where:
- \( d \) = Hydrologic system longitudinal dispersivity (units of length).
- \( v \) = Hydrologic system velocity (units of length per time).
- \( ri \) = retardation factor for nuclide \( i \). This is the ratio of the actual groundwater velocity to effective nuclide velocity and is given for porous media systems as: \((1 + \beta Kd)\) where \( \beta \) is the ratio of the porous media bulk density (mass/volume) divided by the porous media porosity and \( Kd \) is the nuclide...
APPENDIX 2:106

distribution coefficient (volume/mass).

\[ V_i = \frac{v}{r_i} \]

, the effective nuclide convective velocity
( units of length per time) and where \( v \) and \( r_i \) are
defined as in the description of \( D_i \) above.

\[ H_{Li} \]

= The half life of nuclide \( i \) (units of years).

\[ H_{Lj} \]

= The half life of the parent of nuclide \( i \).

\[ A \]

= The natural log. of 0.5 (a constant).

In the direct simulation approach utilized particles of mass (curies) are released from the source areas with weights (curies) as well as times and locations determined by the source description. These particles of mass are then convected according to the effective velocity and time step to a new location. The dispersion process (actually diffusion) is then performed with standard Monte Carlo methods and the final location of all particles at time \( t + \delta t \) is determined. Particle masses are then adjusted for decay and new daughter parcels are created at locations determined from mean daughter and parent effective velocity considerations and time step. This process is then repeated.

An accounting is kept of particle weights crossing the outflow boundary versus time for development of outflow mass versus time curves (concentration versus time curves can be produced by dividing by the fluid outflow rate). Concentration versus distance curves can be generated any time by specifying the resolution desired, adding up the weight (curies) in each spatial cell and dividing by the cell volume thus producing an concentration versus distance curve. This direct simulation approach introduces statistical noise in the solution which must be filtered. Precise solutions are difficult to achieve. However, solutions with sufficient engineering type accuracy (+ or - say 10%) are easily obtained.

1.2 Basic Assumptions
- Uniform one-dimensional steady flow with no coupling between flow and transport (i.e radionuclides are in tracer concentrations.
- Sorption follows a linear isotherm and instantaneous equilibrium is assumed.
- Effective dispersion constant a function of the fluid velocity, media dispersivity and retardation factor.
- Chain decay

1.3 Initial Conditions
**APPENDIX 2:107**

\[ Ni(x,0) = 0 \]

### 1.4 Boundary Conditions

**Inflow:**
- Direct injection or flux boundary condition. The rate of entry of mass (curies) is a user specified function of time (\( B2(F) \)) as described earlier in this report.
- Concentration boundary condition of the B1 type specified earlier in this report.

**Outflow:**
- All outflow boundaries are of the finite discharge type. This is most similar but not equivalent to the E3 type of outflow boundary condition discussed earlier in this text.

This type of outflow boundary allows full convective plus dispersive outflow with no return dispersive flow once the contaminant has crossed the discharge boundary at \( x = L \), where \( L \) is the outflow boundary (i.e. a river or lake). The following diagram illustrates the boundary condition.

```
<table>
<thead>
<tr>
<th>Problem Domain</th>
<th>River or Lake</th>
</tr>
</thead>
<tbody>
<tr>
<td>x=0</td>
<td>(Dispersivity, D ( \neq 0 ))</td>
</tr>
</tbody>
</table>
```

### 1.5 Restrictions To Parameters

- Maximum of nine member chains, 100,000 parcels per contaminant.

### 1.6 Program Language And Size Of Code

The code is written in FLECS which is a structured programming language that produces a FORTRAN source deck from FLECS and FORTRAN source.

The input section of the code contains 1136 statements. The calculational portion contains 1208 statements and the plotting and output analysis section contains 1748 statements.

The code uses a unique disk I/O which makes it operational only on PDP 11/70 series computers.

### 1.7 Applications Of The Code

The code has been routinely used for performance assessment studies for deep geologic repositories.

### 1.8 Availability

The code is available through Pacific Northwest Laboratories.
APPENDIX 2:108

Code: GETOUT

Project Team: Battelle, Pacific Northwest Laboratories, Richland, WA, USA
U.S. Department of Energy

1. Model Characterization

Code: GETOUT

1.1 Equations

GETOUT uses analytical solutions to the equation for one-dimensional solute transport for up to three-member decay chains (Burkholder and Rosinger 1980). This equation may be written:

$$B_i \frac{\partial C_i}{\partial t} = D \frac{\partial^2 C_i}{\partial x^2} - V \frac{\partial C_i}{\partial x} - B_i \lambda_i C_i + B_{i-1} \lambda_{i-1} C_{i-1}$$

where

- $C$ is the concentration
- $B$ is the retardation factor
- $D$ is the dispersion coefficient
- $V$ is the pore velocity
- $\lambda$ is the radioactive decay constant
- $x$ is the position on the travel path

The subscript $i$ refers to the position in the decay chain of an individual radionuclide.

This equation is reduced to analytical solutions for one-, two-, and three-member chains (through a La Place transform technique) subject to a band release boundary condition.

1.2 Basic Assumptions

The principal simplifying assumptions are:

- Sorption follows a linear isotherm and is in instaneous equilibrium.
- All elements have infinite solubility.
- Fluid flow is steady-state.
- A uniform one-dimensional flow path is used.
- Dispersion is axial and the same for all nuclides.
- Radioactivity is released into the ground water through a band release.
- Chain decay with three or less members.

1.3 Initial Conditions

$$C_i(x, 0) = 0.0$$
1.4 Boundary Conditions

Inflow: Radionuclides flow into the system through a band release. Band release assumes that the release is at a constant rate from the time of initial release until the source is depleted. Because decay occurs at the source after the release has started, the nuclide concentrations vary as the release proceeds. The superposition of two step solutions offset by the release duration create the actual band release.

Outflow: $C_j (\infty, t) = \text{finite}$

1.5 Restrictions to Parameters

Retardation coefficients of consecutive nuclides in a chain cannot be equal. Numerical problems are present when simulating large Peclet number cases (i.e. large dispersion).

1.6 Program Language and Size of Code

GETOUT is divided into four FORTRAN IV segments. The system resources on a UNIVAC 11/44 using the EXEC 8 operating system required for each segment are given below.

<table>
<thead>
<tr>
<th>Resource</th>
<th>Program</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>One</td>
</tr>
<tr>
<td>Memory (decimal words)</td>
<td>26,000</td>
</tr>
<tr>
<td>Fortran Statements</td>
<td>3,000</td>
</tr>
<tr>
<td>Execution Time (cp sec)</td>
<td>330</td>
</tr>
<tr>
<td>Mass Storage (words)</td>
<td>205,000</td>
</tr>
<tr>
<td>Number of Subprograms</td>
<td>27</td>
</tr>
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</table>

1.7 Applications of the Code

The code has been used routinely for studies in performance assessment of deep geologic repositories.

1.8 Availability

The code is available through Pacific Northwest Laboratories.
APPENDIX 2:110

Code: UCB-NE-10

Project Team: University of California, Berkeley, CA, USA
U.S. Department of Energy

1. Model Characterization

Code: UCB-NE-10

1.1 Equations

UCB-NE-10 uses analytic solutions to the equation for one-dimensional solute transport for up to three-member decay chains (Harada et al. 1980). This equation may be written:

\[ B_i \frac{\partial C_i}{\partial t} = D \frac{\partial^2 C_i}{\partial x^2} - V \frac{\partial C_i}{\partial x} - B_i \lambda_i C_i + B_{i-1} \lambda_{i-1} C_{i-1} \]

where

- \( C \) is the concentration
- \( B \) is the retardation factor
- \( D \) is the dispersion coefficient
- \( V \) is the pore velocity
- \( \lambda \) is the radioactive decay constant
- \( x \) is the position on the travel path.

The subscripts refer to the position in the decay chain of an individual radionuclide.

This equation is reduced to analytic solutions for one-, two-, and three-member chains (through integration by member) subject to a band release, a step release, or an exponential release boundary condition.

1.2 Basic Assumptions

The principal simplifying assumptions are:

- Sorption follows a linear isotherm and is in instantaneous equilibrium.
- All elements have infinite solubility.
- Fluid flow is steady-state.
- A uniform one-dimensional flow path is used.
- Dispersion is axial and the same for all nuclides.
- Radioactivity is released into the ground water through a band, step, or exponential release.
- Chain decay with three or less members.

1.3 Initial Conditions

\[ C_i(x, 0) = 0.0 \]
1.4 Boundary Conditions

Inflow: Radionuclides flow into the system through a band, step, or exponential release.

Band release assumes that the release is at a constant rate from the time of initial release until the source is depleted. Because decay occurs at the source after the release has started, the nuclide concentrations vary as the release proceeds. The superposition of two-step solutions offset by the release duration create the actual band release.

Exponential release assumes the release rate is a constant proportion of the amount of radionuclides remaining in the waste matrix.

Outflow: \( C_1 (\infty, t) = \text{finite} \)

1.5 Restrictions to parameters

Retardation coefficients of consecutive nuclides in a chain cannot be equal. Numerical problems are present when simulating small Peclet number cases (i.e. small dispersion).

1.6 Program Language and Size of Code

UCB-NE-10 is written in FORTRAN and contains approximately 600 lines of code.

1.7 Applications of the Code

The code has been used in several studies performed by the UCB group.

1.8 Availability

The code is available from the Nuclear Engineering school at UCB.
1. Model Characterization

1.1 Equations

The differential equation solved is:

$$\hat{L}_i N_i(z,t) = K_{i-1} \lambda_{i-1} N_{i-1}(z,t) + \phi_i(z,t)$$

for: \(-\infty < z < \infty\)
\[t > 0\]
\[i = 1, 2, 3, \ldots\]

where the operator \(\hat{L}_i\) is defined as:

$$\hat{L}_i = -D \frac{\partial^2}{\partial z^2} + V \frac{\partial}{\partial z} + K_i \frac{\partial}{\partial t} + \eta_i K_i; \quad V > 0; \quad i = 1, 2, 3, \ldots$$

and where:

- \(z\) is the space coordinate.
- \(t\) represents the time elapsed from the moment at which a contaminating source \(\phi_i(z,t)\) first became active.
- \(i\) is a subscript denoting location within a radioactive decay chain.
- \(N_i(z,t)\) is the concentration of nuclide \(i\) at position \(z\) at time \(t\).
- \(\phi_i(z,t)\) is a general source term for radionuclide \(i\).
- \(D\) is the coefficient of axial dispersion.
- \(K_i\) is the retardation coefficient.
- \(V\) is the water velocity in the \(z\) direction.
- \(\lambda_i\) is the decay constant.
- \(\eta_i\) is defined, for transport with local chemical equilibrium, by \(\eta_i = \frac{\lambda_i}{K_i}\).

1.2 Basic Assumptions

\(D, K,\) and \(V\) are assumed constant.

1.3 Initial Conditions

\(N_i(z,t \leq 0) = 0\) for all \(z\) and \(i\).
1.4 **Boundary Conditions**

\( N_j(z, t) \) and its derivatives tend to zero with a suitable exponent order as \( z \to \pm \infty \).

1.5 **Restrictions to Parameters**

None described in documentation

1.6 **Program Language and Size of Code**

UCB-NE-30 contains approximately 3800 lines of FORTRAN code.

1.7 **Applications of the Code**

The code has been used in several studies performed by the UCB group.

1.8 **Availability**

The code is available from the Nuclear Engineering school at UCB.
APPENDIX 3:1

RESULTS FROM LEVEL 1

<table>
<thead>
<tr>
<th>CASE</th>
<th>PAGE</th>
</tr>
</thead>
<tbody>
<tr>
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<tr>
<td>2</td>
<td>18</td>
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<td>3</td>
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<td>4A</td>
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<td>4B</td>
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<td>6A</td>
<td>88</td>
</tr>
<tr>
<td>6B</td>
<td>95</td>
</tr>
<tr>
<td>7</td>
<td>102</td>
</tr>
</tbody>
</table>
### Case No. 1

**Parameters:** R1, T2, LI, PZ

| CRV Code | 1 TRANSAT | 2 GETOUTO | 3 RANCH | 4 TRCHN | 5 GETOUTY | 6 RANCHY | 7 RANCH | 8 METIS | 9UCR-HX | 10 HWTY | 11 TRANSAT | 12 HWTIDPFLB | 13 COLUMN | 14 PURLFO | 15 SWENT | 16 TRANSAT | 17 UCRR-NX | 18 SWIFT | 19 RANCH | 20 CESD | 21 METIS | 22 BPCF | 23 HUTBAR | 24 HWT/DWYB | 25 SWIFT | 26 SWIFT | 27 SWENT | 28 HWTIDPFLB |
|----------|----------|----------|--------|--------|----------|---------|--------|--------|--------|--------|----------|-----------|---------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
|          | B1E1     | B1E1     |        | B1E1   | B1E1     | B1E1    | B1E1   | B1E1   | B1E1   | B1E1   | B1E1     | B1E1      | B1E1    | B1E1   | B1E1   | B1E1   | B1E1   | B1E1   | B1E1   | B1E1   | B1E1   | B1E1   | B1E1   | B1E1   |
| C Max    | 168000   | 165000   | 167000 | 16500  | 175000   | 16500   | 16500  | 17100  | 16400  | 150000 | 158000   | 161000    | 160000  | 16000  | 175000 | 177000 | 18200  | 18000 | 17100 | 175000 | 190000 | 183000 | 175000 | 175000 | 168000 |
| T(CMAX)  | 66400    | 0        | 67200  | 67200  | 66600    | 67200   | 67200  | 68200  | 67300  | 0      | 63300    | 62300     | 60600   | 60600  | 30900  | 72800  | 72800  | 76800 | 30040 | 73700 | 173000 | 84000  | 36600  | 36400  | 65400  |
| T+(10.I) | 0        | 328000   | 330000 | 328000 | 332000   | 330000  | 330000 | 346000 | 339000 | 0      | 308000   | 304000    | 304000  | 304000 | 304000 | 304000 | 304000 | 304000 | 304000 | 304000 | 304000 | 304000 | 304000 |
| T-(10.I) | 0        | 328000   | 330000 | 328000 | 332000   | 330000  | 330000 | 346000 | 339000 | 0      | 308000   | 304000    | 304000  | 304000 | 304000 | 304000 | 304000 | 304000 | 304000 | 304000 | 304000 | 304000 | 304000 |
| C Max    | 317000   | 94500    | 288000 | 230000 | 288000   | 292000  | 292000 | 237000 | 295000 | 0      | 255000   | 87800     | 236000  | 87900  | 94300  | 94300  | 94300  | 94300  | 94300  | 94300  | 94300  | 94300  | 94300  |
| T(CMAX)  | 572000   | 554000   | 69400  | 91200   | 93800    | 95400   | 95400  | 96300  | 96600  | 0      | 95700    | 53300     | 75400   | 75400  | 53500  | 53500  | 53500  | 53500  | 53500  | 53500  | 53500  | 53500  | 53500  |
| T+(10.I) | 572000   | 554000   | 69400  | 91200   | 93800    | 95400   | 95400  | 96300  | 96600  | 0      | 95700    | 53300     | 75400   | 75400  | 53500  | 53500  | 53500  | 53500  | 53500  | 53500  | 53500  | 53500  | 53500  |
| T-(10.I) | 572000   | 554000   | 69400  | 91200   | 93800    | 95400   | 95400  | 96300  | 96600  | 0      | 95700    | 53300     | 75400   | 75400  | 53500  | 53500  | 53500  | 53500  | 53500  | 53500  | 53500  | 53500  | 53500  |

**Appendix 3-12**

**Retention Calculated with Matrix Diffusion**

**MAX TIME (YR)**: 2.50E+05
**ARITHM. OPER.**: 9.34E+07
**OPERATIONS/YR**: 3.74E+02

**Remarks**:
- TRANSAT: 2.50E+05
- GETOUTO: 2.22E+06
- RANCH: 2.09E+06
- TRCHN: 5.07E+05
- GETOUTY: 2.03E+06
- TROUGH: 5.00E+05
- RANCHY: 8.00E+05
- METIS: 5.00E+05
- UCB-NX: 2.20E+06
- HWTY: 6.00E+05
- TRANSAT: 2.44E+05
- HWTIDPFLB: 7.99E+05
- COLUMN: 2.20E+06
- PORYLO: 6.00E+05
- SWENT: 2.42E+05
- TRANSAT: 2.44E+05
- UCRR-NX: 2.20E+06
- SWIFT: 1.00E+06
- RANCH: 2.21E+06
- GEOS: 2.20E+06
- METIS: 5.00E+05
- BPCF: 6.00E+05
- HUTBAR: 1.40E+06
- HWT/DWYB: 1.00E+06
- SWIFT: 4.99E+05
- DRAKA: 8.40E+05
- SWENT: 2.37E+05

**Retention Calculated with Matrix Diffusion**
APPENDIX 3.3

INTRACOIN CASE 1 PARAMETERS: N1R1 T2 L1 P2
NUCLEIDE 1

Time (Years)

Concentration in outflow (act./ln.)
APPENDIX 3:4

INTRACOIN CASE 1 PARAMETERS: R1 T2 L1 P2
NUCLIDE 2

[Graphs showing concentration in outflow over time (Years).]
INTRACON CASE 1 PARAMETERS: R1 T2 L1 P2
NUCLIDE 3

APPENDIX 3:5

[Graphs showing concentration in outflow vs. time in years with logarithmic scale, indicating data points and curves for different nuclides over varying time periods.]
### APPENDIX 3:6

#### CASE NO 1

### PARAMETERS

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>8.15%</td>
</tr>
</tbody>
</table>

#### NUCLIDE 1

<table>
<thead>
<tr>
<th>Code</th>
<th>C_max</th>
<th>T(cmax)</th>
<th>T+(10.1)</th>
<th>T-(10.1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>8.15%</td>
<td>8.15%</td>
<td>8.15%</td>
<td>8.15%</td>
</tr>
</tbody>
</table>

#### NUCLIDE 2

<table>
<thead>
<tr>
<th>Code</th>
<th>C_max</th>
<th>T(cmax)</th>
<th>T+(10.1)</th>
<th>T-(10.1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>8.15%</td>
<td>8.15%</td>
<td>8.15%</td>
<td>8.15%</td>
</tr>
</tbody>
</table>

#### NUCLIDE 3

<table>
<thead>
<tr>
<th>Code</th>
<th>C_max</th>
<th>T(cmax)</th>
<th>T+(10.1)</th>
<th>T-(10.1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>8.15%</td>
<td>8.15%</td>
<td>8.15%</td>
<td>8.15%</td>
</tr>
</tbody>
</table>

---

### MAX TIME (YR) ARITHM. OPER. OPERATIONS/YR

<table>
<thead>
<tr>
<th>Code</th>
<th>Time</th>
<th>Operations/Yr</th>
</tr>
</thead>
<tbody>
<tr>
<td>TRANSA</td>
<td>1.25</td>
<td>1.88</td>
</tr>
<tr>
<td>GETDO</td>
<td>9.77</td>
<td>8.02</td>
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<td>RANCH</td>
<td>1.04</td>
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<tr>
<td>TROUGH</td>
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<td>COLUMN</td>
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<tr>
<td>GEOS</td>
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<tr>
<td>METIS</td>
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<tr>
<td>DRAMA</td>
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</tr>
<tr>
<td>WNT1DFNL</td>
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</tr>
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</table>
APPENDIX 3:7

INTRACOIN CASE 1 Parameters: II R2 T2 L1 P2

NUCLEIDE 1

<table>
<thead>
<tr>
<th>Time (Years)</th>
<th>Concentration in outflow (act. m.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10^3</td>
<td>10^6</td>
</tr>
<tr>
<td>10^4</td>
<td>10^7</td>
</tr>
<tr>
<td>10^5</td>
<td>10^8</td>
</tr>
<tr>
<td>10^6</td>
<td>10^9</td>
</tr>
</tbody>
</table>

Time (Years)
APPENDIX 3:8

INTRACOIN CASE 1 PARAMETERS: II R2 T2 L1 P2
NUCLIDE 2
APPENDIX 3:9

INTRACOIN CASE 1 PARAMETERS: II R2 T2 L1 P2
NUCLEIDE 3
### Case No. 1

**Parameters I2 B1 T2 L1 P2**

<table>
<thead>
<tr>
<th>Nuclide 1</th>
<th>Nuclide 2</th>
<th>Nuclide 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>CRY Cuda</td>
<td>C MAX T(1CMAX) T+5(10.1) T-5(10.1)</td>
<td>C MAX T(1CMAX) T+5(10.1) T-5(10.1)</td>
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<tr>
<td>1 GETOUTO B1E1</td>
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<td>0</td>
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<td>2 TRUNCH B1E1</td>
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<td>0</td>
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<tr>
<td>3 GETOUTY B1E1</td>
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<td>0</td>
</tr>
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<td>4 TRUNCH B1E1</td>
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<td>0</td>
</tr>
<tr>
<td>5 RANCH B1E1</td>
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<td>0</td>
</tr>
<tr>
<td>6 RANCH B1E1</td>
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<td>0</td>
</tr>
<tr>
<td>7 METIS B1E1</td>
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<td>0</td>
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<td>8 UCN-HX B1E1</td>
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<td>0</td>
</tr>
<tr>
<td>10 NMTDPMLB2E3</td>
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<td>0</td>
</tr>
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</tr>
<tr>
<td>12 PORPLO B1E3</td>
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</tr>
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<td>13 UCN-HX B2E1</td>
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</tr>
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</tr>
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<td>0</td>
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APPENDIX 3:11

INTRACOIN CASE 1 PARAMETERS: I2 R1 T2 L1 P2
NUCLIDE 1
APPENDIX 3:12

INTRACOIN CASE 1 PARAMETERS: 12 R1 T2 L1 P2
NUCLIDE 2

Concentration in outflow (act.un.)

Time (Years)

10^0 10^1 10^2 10^3 10^4 10^5

10^-3 10^-4 10^-5 10^-6 10^-7 10^-8

Concentration in outflow (act.un.)

Time (Years)

10^0 10^1 10^2 10^3 10^4 10^5

10^-3 10^-4 10^-5 10^-6 10^-7 10^-8
APPENDIX 3:13

INTRACOIN CASE 1 PARAMETERS: I2 R1 T2 L1 P2
NUCLEIDE 3
### APPENDIX 3:14

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APPENDIX 3:16

INTRACOIN CASE 1 PARAMETERS: 02 R2 T2 L1 P2
NUCLEIDE 2

Time (Years)

Concentration in outflow (act./ln.)

Concentration in outflow (act./ln.)
APPENDIX 3:17

INTRACOIN CASE 1 PARAMETERS: 12 R2 T2 L1 P2
NUCLIDE 3

Time (Years)

Concentration in outflow (act.u.)

Time (Years)
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Retention calculated with matrix diffusion.
APPENDIX 3:19

INTRACOIN CASE 2 PARAMETERS: R1, R2, L1, P2
NUCLIDE 1

[Graph showing concentration in outflow (actum) versus time (years).]
APPENDIX 3:20

INTRACOIN CASE 2 PARAMETERS: R1 T2 L1 P2
NUCLIDE 2

[Graph showing concentration in outflow over time (years) with various curves labeled 1 to 18.]
APPENDIX 3:21

INTRACOIN CASE 2 PARAMETERS: N1 R1 T2 L1 P2
NUCLEIDE 3
## APPENDIX 3:22

**CASE NO 2**

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APPENDIX 3:23

INTRACOIN CASE 2 PARAMETERS: \( \mathbf{R}_2 \mathbf{T}_2 \mathbf{L}_1 \mathbf{P}_2 \)

NUCLEIDE 1

*Concentration in outflow (act./n) vs Time (Years)*

---

*Concentration in outflow (act./n) vs Time (Years)*
APPENDIX 3:25

INTRACOIN CASE 2 PARAMETERS: R2 T2 L1 P2
NUCLEIDE 3

[Graph showing concentration in outflow versus time (years) with multiple curves labeled 1 to 14.]

[Another graph showing concentration in outflow versus time (years) with multiple curves labeled 1 to 14.]
## Case No 2

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APPENDIX 3:27

INTRANOD CASE 2 PARAMETERS: I2 R1 T2 L1 P2
NUCLEIDE 1
INTRACOIN CASE 2  PARAMETERS: 12 R1 T2 L1 P2
NUCLEIDE 2
### APPENDIX 3:30

**CASE NO 2**

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APPENDIX 3:31

INTRACOIN CASE 2 PARAMETERS: I2 R2 T2 L1 P2
NUCLEIDE 1
APPENDIX 3:32

INTRACTONE CASE 2  PARAMETERS: 12 R2 T2 L1 P2
NUCLEIDE 2
APPENDIX 3:33

INTRACOIN CASE 2 PARAMETERS: I2 R2 T2 L1 P2
NUCLEIDE 3

Graph showing concentration in outflow (actun) vs time (years) with various curves labeled from 1 to 12.
**CASE NO 3**

**PARAMETERS 11 R1 T2 L1 P2**

| CRV CODE | NUCLIDE 1 | | | | NUCLIDE 2 | | | | | NUCLIDE 3 | | | | |
|----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
|          | C MAX     | T(CMAX)   | T+(10.1)  | T-(10.1)  | C MAX     | T(CMAX)   | T+(10.1)  | T-(10.1)  | C MAX     | T(CMAX)   | T+(10.1)  | T-(10.1)  |
| 1 TRUChN| 3.59E-06  | 176000    | 69100     | 344000    | 3.29E-08  | 245000    | 99200     | 571000    | 6.59E-08  | 246000    | 102000    | 577000    |
| 2 MNTDPMLB1| 3.47E-06  | 172000    | 72300     | 354000    | 3.79E-08  | 225000    | 88800     | 563000    | 4.75E-08  | 241000    | 99200     | 577000    |
| 3 COLUMN| 3.73E-06  | 172000    | 73300     | 341000    | 3.34E-08  | 248000    | 101000    | 566000    | 6.68E-08  | 240000    | 103000    | 576000    |
| 4 SWIFT | 3.02E-06  | 194000    | 85100     | 389000    | 2.84E-08  | 265000    | 115000    | 0         | 5.70E-08  | 267000    | 117000    | 0         |
| 5 GEOS  | 2.40E-06  | 200000    | 87400     | 395000    | 2.27E-08  | 270000    | 117000    | 616000    | 4.54E-08  | 270000    | 120000    | 610000    |
| 6 SWENT| 2.97E-06  | 194000    | 83400     | 394000    | 2.80E-08  | 266000    | 114000    | 0         | 5.63E-08  | 269000    | 117000    | 0         |
| 7 DFCT  | 2.80E-06  | 195000    | 84700     | 0         | 0         | 0         | 0         | 0         | 0         | 0         | 0         | 0         |
| 8 WFT/DVM| 2.58E-06  | 211000    | 99100     | 404000    | 6.30E-08  | 266000    | 112000    | 579000    | 8.87E-08  | 270000    | 127000    | 584000    |
| 9 SWIFT | 3.01E-06  | 193000    | 85000     | 390000    | 2.84E-08  | 264000    | 115000    | 0         | 5.69E-08  | 268000    | 117000    | 0         |
| 10 DRAMA| 3.11E-06  | 211000    | 80500     | 378000    | 6.92E-08  | 242000    | 89800     | 481000    | 5.33E-08  | 242000    | 99800     | 571000    |
| 11 SWENT| 3.10E-06  | 190000    | 78800     | 384000    | 2.90E-08  | 260000    | 108000    | 0         | 5.80E-08  | 260000    | 111000    | 0         |

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APPENDIX 3:36

INTRACOIN CASE 3 PARAMETERS: II R1 T2 L1 P2
NUCLEIDE 2

[Graphs showing concentration in outflow over time (years)]

[Graphs showing concentration in outflow over time (years)]
APPENDIX 3:37

INTRACOM CASE 3 PARAMETERS: R1 T2 L1 P2 NUCLIDE 3
### **APPENDIX 3:38**

**U Of J**

---

**PARAMETERS T1 R2 T2 L1 P2**

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**MAX TIME (yr)**

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INTRACOIN CASE 3 PARAMETERS: \( R_2 \) \( T_2 \) \( L_1 \) \( P_2 \)

NUCLIDE 1

![Graph showing concentration in outflow over time](image-url)
APPENDIX 3:40

INTRACOIN CASE 3 PARAMETERS: R2 T2 L1 P2
NUCLEIDE 2

Graphs showing concentration in outflow (act./ln.) versus time (years). Two graphs are present, each depicting the same relationship between concentration and time for different scenarios or conditions, indicated by the numbers 1 to 6. The graphs are used to illustrate the behavior of the nuclide over time under varying conditions.
APPENDIX 3:41

INTRACOIN CASE 3 PARAMETERS: I1 R2 T2 L1 P2 NUCLIDE 3

[Graphs showing concentration in outflow versus time (years)]

Concentration in outflow (act.u.)

Time (Years)

Concentration in outflow (act.u.)

Time (Years)
### APPENDIX 3

**CASE NO 3**

**PARAMETERS**

- $I_2$, $R_1$, $T_2$, $L_1$, $P_2$

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INTRACOIN CASE 3 PARAMETERS: R2 R1 T2 L1 P2
NUCLEIDE 1
APPENDIX 3:44

INTRACOIN CASE 3 PARAMETERS: L2 R1 T2 L1 P2
NUCLIDE 2

[Graph showing concentration in outflow over time for different cases labeled 1 to 6.]

[Graph showing concentration in outflow over time for different cases labeled 1 to 6.]
APPENDIX 3:45

INTRACOIN CASE 3 PARAMETERS: l2 R1 T2 L1 P2
NUCLEIDE 3

[Graph showing concentration in outflow over time (years).]

[Another graph showing concentration in outflow over time (years).]
## Case No 3

### Parameters I2 R2 T2 L1 P2

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APPENDIX 3:47

INTRACOIN CASE 3 PARAMETERS: I2 R2 T2 L1 P2
NUCLIDE 1

![Graph showing concentration in outflow (act.n.) over time (years).]
APPENDIX 3:48

INTRACOIN CASE 3 PARAMETERS: L2 R2 T2 L1 P2
NUCLEIDE 2

Time (Years)

Concentration in outflow (act.l/n)

$10^{-8}$

$10^{-7}$

$10^{-6}$

$10^{-5}$

$10^{-4}$

$10^{-3}$

$10^{-2}$

$10^{-1}$

$10^0$

$10^1$

$10^2$

$10^3$

$10^4$

$10^5$

$10^6$

$10^7$

Time (Years)
INTRACOIN CASE 3

PARAMETERS: L2 R2 T2 L1 P2

NUCLEIDE 3

Concentration in outflow (act. trn.)

Time (Years)

Concentration in outflow (act. trn.)

Time (Years)
### APPENDIX 3:50

**CASE NO 4A**

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<th>REMARKS</th>
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</table>
APPENDIX 3:51

INTRACOIN CASE 4A PARAMETERS: \( R_2 \), \( T_2 \), \( L_1 \), \( P_2 \)

NUCLEIDE 1

![Graph showing activity outflow over time in years.](image-url)
APPENDIX 3:52

INTRACOIN CASE 4A PARAMETERS: I1 R2 T2 L1 P2
NUCLIDE 2

Activity outflow (act.un. / year)

Time (Years)

Activity outflow (act.un. / year)

Time (Years)
## APPENDIX 3:54

### M E O 4A

**parameters:** 15 B2 T 3 P2

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<th>Operations/yr</th>
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APPENDIX 3:54
INTRACOHS CASE 4A PARAMETERS: $G_4, T_2, T_1, P_2$
NUCLEID 1
APPENDIX 3:56

INTRACOIN CASE 4A PARAMETERS: T1 R2 T2 L1 F2
NUCLIDE 2

Graph with concentration in outflow on the y-axis and Y-coordinate (m) on the x-axis.
INTRACOIN CASE 4A PARAMETERS: H R2 T2 L1 P2
NUCLIDE 3
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APPENDIX 3:59

INTRACOIN CASE 4A PARAMETERS: I2 R T2 L1 P2
NUCLEIDE 1
APPENDIX 3:60

INTRACOIN CASE 4A PARAMETERS: l2 R2 T2 L1 P2

NUCLIDE 2

![Graph 1](image1)

![Graph 2](image2)
APPENDIX 3:61

INTRACOIN CASE 4A PARAMETERS: \( I_2 \ R_2 \ T_2 \ L_1 \ P_2 \)

NUCLEIDE 3

Activity outflow (act. u. / year)

Time (Years)

Activity outflow (act. u. / year)

Time (Years)
**APPENDIX 3:62**

**CASE NO 4A**

**PARAMETERS** I2 B2 T2 L1 P2

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<td>3 MEIT8</td>
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APPENDIX 3:62
APPENDIX 3:64

INTRACOIN CASE 4A PARAMETERS: \( R_2 \), \( R_2 \), \( T_2 \), \( L_1 \), \( P_2 \)

NUCLIDE 2

Graphs showing concentration in outflow (act.u.) vs. Y-coordinate (m) for different cases.
APPENDIX 3:65

INTRACON CASE 4A PARAMETERS: 12 R2 T2 L1 P2
NUCLEIDE 3

Concentration in outflow (act. u.)

Y-coordinate (m)

Concentration in outflow (act. u.)

Y-coordinate (m)
### Case No 48

**Parameters I1 R2 T2 L1 P2**

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<th>T(PMAX)</th>
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**Remarks**

### Case No 48

**Parameters I1 R2 T2 L1 P2**

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<th>Y MAX</th>
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<th>Remarks</th>
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**Remarks**
APPENDIX 3:67

INTRACON CASE 48 PARAMETERS: II R2 T2 L1 P2
NUCLIDE 1
APPENDIX 3:68

INTRACOIN CASE 48 PARAMETERS: 11 R 2 T 2 L 1 P 2
NUCLEIDE  2

10^-6

10^-4

10^-2

10^-1

Time (Years)

Activity outflow (act.u.n. / year)

1

2

10^0

10^1

10^2

10^3

10^4

5 10^4

10^3

Time (Years)

Activity outflow (act.u.n. / year)

1

2

10^0

10^-1
APPENDIX 3:70

INTRACOIN CASE 48 PARAMETERS: II R2 T2 L1 P2
NUCLEIDE 1

[Graphs showing concentration in outflow (act.un.) vs. Y-coordinate (m)]
APPENDIX 3:71

INTRACOIN CASE 4B PARAMETERS: R1 R2 T2 L1 P2
NUCLEIDE 2

Concentration in outflow (act. pm)

Y-coordinate (m)

Concentration in outflow (act. pm)

Y-coordinate (m)
INTRACON CASE 4B PARAMETERS: N2 R2 T2 L1 P2
NUCLIDE 3

Concentration in outflow (act. um)

Y-coordinate (m)

10^{-9} 10^{-8} 10^{-7} 10^{-6} 10^{-5} 10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{1} 10^{2} 10^{3} 10^{4}
### Case No. 4B

#### Parameters I2 R2 T2 L1 P2

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<th>Remarks</th>
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### Code

- SWIFT II B2E1

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### Case No. 4B

#### Parameters I2 R2 T2 L1 P2

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<table>
<thead>
<tr>
<th>MAX Time (Yr)</th>
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### Code

- SWIFT II B2E1

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### Parameters I2 R2 T2 L1 P2

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<tbody>
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### Code

- SWIFT II B2E1

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### Parameters I2 R2 T2 L1 P2

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- SWIFT II B2E1

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### Parameters I2 R2 T2 L1 P2

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- SWIFT II B2E1

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- SWIFT II B2E1
INTRACON CASE 4B PARAMETERS: I2 R2 T2 L1 P2
NUCLIDE 1

[Graph showing the activity outflow vs. time in years for different nuclides.]
APPENDIX 3:75

INTRACOM CASE 48 PARAMETERS: L2 R2 T2 L1 P2
NUCLEIDE 2

Diagram 1:

Activity outflow (act. u/n. / year) vs. Time (Years)

Diagram 2:

Activity outflow (act. u/n. / year) vs. Time (Years)
APPENDIX 3:76

INTRACOM CASE 48 PARAMETERS: $I_2 R_2 T_2 L_1 P_2$
NUCLIDE 3

Graph 1:
Activity outflow (actu./year)

Graph 2:
Activity outflow (actu./year)
INTRACOIN CASE 4B PARAMETERS: I2 P2 T2 L1 P2
NUCLIDE 1

**Graph 1:**
- **Y-axis:** Concentration in outflow (act.un.)
- **X-axis:** Y-coordinate (m)

**Graph 2:**
- **Y-axis:** Concentration in outflow (act.un.)
- **X-axis:** Y-coordinate (m)
INTRACOIN CASE 4B PARAMETERS: I2 R2 T2 L1 P2
NUCLEIDE 3
**CASE NO 5**

**PARAMETERS**

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**MAX TIME (YR)**

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**REMARKS**

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APPENDIX 3:80
APPENDIX 3:81

INTRACOIN CASE 5 PARAMETERS: II RO T2 L1 P2
NUCLEIDE 1

Graph 1:
- Concentration in outflow (act.u.n.)
- Time (Years)

Graph 2:
- Concentration in outflow (act.u.n.)
- Time (Years)
APPENDIX 3:82

INTRACOIN CASE 5 PARAMETERS: R0 T2 L1 P2
NUCLEIDE 2

Concentration in outflow (act./un.)

Time (Years)

Concentration in outflow (act./un.)

Time (Years)
APPENDIX 3:83

INTRACOIN CASE 5 PARAMETERS: N RO T2 L1 P2
NUCLEIDE 3

Graph 1: Concentration in outflow (act./l.m.) vs. Time (Years)

Graph 2: Concentration in outflow (act./l.m.) vs. Time (Years)
# Case No. 5

**Parameters** T1 R0 T2 L1 P2

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B1 UNTIL T. THEREAFTER d=DC/DE=Q*C AT THE FRONT END
APPENDIX 3:85

INTRACOIN CASE 5 PARAMETERS: Q2 RO T2 L1 P2
NUCLIDE 1

![Graph showing the concentration in outflow as a function of time (years)]
APPENDIX 3:86

INTRACOIN CASE 5 PARAMETERS: l2 R0 T2 L1 P2
NUCLIDE 2

[Graph showing concentration in outflow over time (years).]
APPENDIX 3:87

INTRACOIN CASE 5 PARAMETERS: I2 RO T2 L1 P2
NUCLIDE 3

[Graph depicting concentration in outflow over time (years)]

[Graph depicting concentration in outflow over time (years)]
### **CASE NO 6A**

**PARAMETERS 12 RO T2 L1 P2**

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### **CASE NO 6A**

**PARAMETERS 12 RO T2 L1 P2**

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**REMARKS**

- AT=5M, FLOW REGION 600M*500M
- TMAX(HF237)= 9.024+05, TMAX(U233)= 7.024+05
- AT=5M, FLOW REGION= 600M * 100M, TMAX(HF237)= 9.024+5, TMAX(U233)=
APPENDIX 3:89

INTRACON CASE 6A PARAMETERS: L2 R0 T2 L1 P2
NUCLEIDE 1
INTRACOIN CASE 6A PARAMETERS: 62 R0 T2 L1 P2
NUCLIDE 2

Time (Years)

Concentration in outflow (act.un.)

Time (Years)
APPENDIX 3:91

INTRACOIN CASE 6A PARAMETERS: 12 R0 T2 L1 P2
NUCLIDE 3
INTRACOIN CASE 6A PARAMETERS: I2 R0 T2 L1 P2
NUCLIDE 1
INTRACOIN CASE 6A PARAMETERS: 12 R0 T2 L1 P2
NUCLEIDE 2
APPENDIX 3:94

INTRACOIN CASE 6A PARAMETERS: 12 RO T2 L1 P2
NUCLEIDE 3

[Graph showing Concentration in outflow vs Y-coordinate (m)]
### CASE NO 6B

#### PARAMETERS 12 B0 T2 L1 P2

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OUTFLOW LOCATION X= 0M, AT= 5M
INTRACON CASE 6B PARAMETERS: I2 R0 T2 L1 P2
NUCLEIDE 1
APPENDIX 3:97

INTRACOIN CASE 6B PARAMETERS: 12 R0 T2 L1 P2
NUCLEIDE 2

[Graph 1: Concentration in outflow vs. Time (Years)
- Log scale on both axes
- Three curves labeled 1, 2, and 3]

[Graph 2: Concentration in outflow vs. Time (Years)
- Log scale and linear scale on separate axes
- Curve labeled 2]
INTRACOIN CASE 68 PARAMETERS: \( \alpha \) \( 0 \) \( T2 \) \( L1 \) \( P2 \)

NUCLEIDE 3

![Graph](image-url)
APPENDIX 3:99

INTRACOIN CASE 6B PARAMETERS: I2 R0 T2 L1 P2
NUCLEIDE 1

10^{-9}

10^{-8}

10^{-7}

10^{-6}

10^{-5}

10^{-4}

10^{-3}

10^{-2}

Y-coordinate (m)

Concentration in outflow (act.un.)

1

1

1

6 \times 10^{-2}

10^{-1}

10^{0}

10^{1}

10^{2}

10^{3}

Y-coordinate (m)

Concentration in outflow (act.un.)
INTRACOIN CASE 6B PARAMETERS: I2 R0 T2 L1 P2
NUCLIDE 2

Concentration in outflow (act/ln l)

Y-coordinate (m)

Concentration in outflow (act/ln l)

Y-coordinate (m)
APPENDIX 3:101

INTRACOIN CASE 68 PARAMETERS: l2 R0 T2 L1 P2
NUCLEIDE 3

[Graph showing concentration in outflow vs Y-coordinate (m)]

1. Concentration in outflow (act.un.)
2. Y-coordinate (m)

[Graph showing concentration in outflow vs Y-coordinate (m)]

1. Concentration in outflow (act.un.)
2. Y-coordinate (m)
PARAMETERS I1 R1 T2 L1 P2

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MAX TIME (YR)  ARITH. OPER.  OPERATIONS/YR  REMARKS

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APPENDIX 3:103

INTRACOIN CASE 7 PARAMETERS: II R1 T2 L1 P2
NUCLEIDE 1

Time (Years)
INTRACOIN CASE 7 PARAMETERS: N1 R1 T2 L1 P2
NUCLIDE 2

Time (Years)

Concentration in outflow (act.un.)

10^{-6} 10^{-3} 10^{0} 10^{3} 10^{6}

10^{-6} 10^{-3} 10^{0} 10^{3} 10^{6}

4 \times 10^{4} 10^{5}
APPENDIX 3:105

INTRACOIN CASE 7 PARAMETERS: II R1 T2 L1 P2
NUCLIDE 3

PARAMETERS:

- kma = 1.0E-4
- kma = 1.0E-5
- kma = 1.0E-2
- kma = 1.0E-3
- kma = 1.0E+5

Time (Years)

Concentration in outflow (act.l.u.)
### Parameters 11 12 13 12 12 12

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#### Max Time (Yr) Arithm. Oper. Operations/Yr

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APPENDIX 3:107

INTRACOIN CASE 7 PARAMETERS: II R2 T2 L1 P2
NUCLEIDE 1

[Graph showing concentration in outflow (act.un.) vs. time (years) with various kma values indicated on each curve.]
APPENDIX 3:108

INTRACOIN CASE 7 PARAMETERS: N1 R2 T2 L1 P2
NUCLEIDE 2

(Time (Years)

Concentration in outflow (act.un.)

N1 kma = 1.0E-4
R2 kma = 1.0E-5
T2 kma = infinity
L1 kma = 1.0E-2
P2 kma = 1.0E-5

(Time (Years)

Concentration in outflow (act.un.)

N1 kma = 1.0E-5
R2 kma = 1.0E-4
T2 kma = 1.0E-2
L1 kma = 1.0E-5
P2 kma = 1.0E+5
APPENDIX 3:109

INTRACON CASE 7 PARAMETERS: R2 T2 L1 P2
NUCLEIDE 3

CONCENTRATION in outflow (act. units)

Time (Years)

10

10

10

10
### APPENDIX 3.3

**PARAMETERS 12 E1 T2 L1 P2**

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**MAX TIME (YR) ARITHM. OPER. OPERATIONS/yr REMARKS**

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<th>B1E1</th>
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<th>3.35E+08</th>
<th>3.31E+03</th>
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INTRACOIN CASE 7 PARAMETERS: R1 T2 L1 P2
NUCLEIDE 1

Time (Years)

Concentration in outflow (act.un.)

0
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}

10^{3}

kma = 1.0E-5
kma = 0
kma = 1.0E-6
kma = 1.0E-4

Time (Years)

10^{3}
10^{4}
10^{5}
10^{6}
10^{7}
10^{8}

10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}

kma = 1.0E-5
kma = 0
kma = 1.0E-4

Concentration in outflow (act.un.)

0
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}

10^{3}

kma = 1.0E-5
kma = 0
kma = 1.0E-6
kma = 1.0E-4
APPENDIX 3:112

INTRACOIN CASE 7 PARAMETERS: 12 R1 T2 L1 P2
NUCLEIDE 2

[Graph showing concentration in outflow (act. u.) vs. time (years) for different values of kma.]

12 kma = 1.0E-2
11 kma = 0
10 kma = 1.0E-5
9 kma = 1.0E-4
8 kma = 1.0E-2
7 kma = 1.0E-5
6 kma = 1.0E-4
5 kma = 1.0E-5
4 kma = 1.0E-4
3 kma = 1.0E-5
2 kma = 1.0E-4
1 kma = 1.0E-5
0 kma = 1.0E-4
APPENDIX 3:113

INTRACTION CASE 7 PARAMETERS: I2 R1 T2 L1 P2
NUCLIDE 3

![Graph showing concentration in outflow as a function of time for different values of kma. The graph includes curves for kma = 1.0E-5, 1.0E-4, 1.0E-3, 1.0E-2, and 1.0E+5. The x-axis represents time in years, ranging from $10^3$ to $10^8$, and the y-axis represents concentration in outflow (act.luhn).]
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APPENDIX 3:115

INTRACOIN CASE 7 PARAMETERS: I2 R2 T2 L1 P2
NUCLIDE 1

---

**Concentration in outflow (act.un.)**

**Time (Years)**

---

**Concentration in outflow (act.un.)**

**Time (Years)**
INTRACOIN CASE 7 PARAMETERS: I2 R2 T2 L1 P2
NUCLIDE 2

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</table>

Time (Years) vs. Concentration in outflow (act.un.)

Time (Years) vs. Concentration in outflow (act.un.)
INTRACOIN Parties (in alphabetic order):

Atomic Energy of Canada Ltd (Canada), Commissariat à l’Énergie Atomique/Institut de Protection et de Sûreté Nucléaire (France), Nationale Genossenschaft fur die Lagerung Radioaktiver Abfälle (Switzerland), National Radiological Protection Board (U.K.), Projekt Sicherheitsstudien Entsorgung (Federal Republic of Germany), Swedish Nuclear Fuel Supply Co. (Sweden), Swedish Nuclear Power Inspectorate (Sweden), Technical Research Centre of Finland (Finland), U.K. Atomic Energy Authority/Atomic Energy Research Establishment (U.K.), U.S. Department of Energy (USA), U.S. Nuclear Regulatory Commission (USA).

Project secretariat: Swedish Nuclear Power Inspectorate, Kemakta Consultants Co. Swiss Federal Institute for Reactor Research

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