

Nagra

Nationale
Genossenschaft
für die Lagerung
radioaktiver Abfälle

Cédra

Société coopérative
nationale
pour l'entreposage
de déchets radioactifs

Cisra

Società cooperativa
nazionale
per l'immagazzinamento
di scorie radioattive



TECHNICAL REPORT 85-38

TROUGH – 1 D
A one-dimensional computer code for
calculation of radionuclide transport
in groundwater

D. J. Gilby
R. J. Hopkirk

February 1985

Polydynamics Ltd, Zürich

Nagra

Nationale
Genossenschaft
für die Lagerung
radioaktiver Abfälle

Cédra

Société coopérative
nationale
pour l'entreposage
de déchets radioactifs

Cisra

Società cooperativa
nazionale
per l'immagazzinamento
di scorie radioattive

TECHNICAL REPORT 85-38

TROUGH – 1 D

A one-dimensional computer code for
calculation of radionuclide transport
in groundwater

D. J. Gilby
R. J. Hopkirk

February 1985

Polydynamics Ltd, Zürich

Der vorliegende Bericht wurde im Auftrag der Nagra erstellt.
Die Autoren haben ihre eigenen Ansichten und Schlussfolgerungen dargestellt. Diese müssen nicht unbedingt mit denjenigen der Nagra übereinstimmen.

Le présent rapport a été préparé sur demande de la Cédra.
Les opinions et conclusions présentées sont celles des auteurs et ne correspondent pas nécessairement à celles de la Cédra.

This report was prepared as an account of work sponsored by Nagra. The viewpoints presented and conclusions reached are those of the author(s) and do not necessarily represent those of Nagra.

A C K N O W L E D G E M E N T S

The computer code described in this report has been created and developed with the combined financial support of NAGRA in Switzerland and the National Radiation Protection Board (NRPB) of the United Kingdom.

The authors wish to thank in particular Dr. Charles Mc Combie at NAGRA and Ms. Marion Hill at NRPB for their support and encouragement.

A B S T R A C T

A family of computer codes with the generic name TROUGH (Transport of Radioactive Outflows in Underground Hydrology) has been produced for the safety analysis of radioactive waste repositories. The simplest version of this family, TROUGH-1D, has undergone thorough development and testing and has been applied to several aspects of the NAGRA work. This present report contains a technical description and user manual for the code.

Z U S A M M E N F A S S U N G

Für die Sicherheitsanalyse der Endlager für nukleare Abfälle wurde eine Gruppe von Computerprogrammen mit dem generischen Namen TROUGH (Transport of Radioactive Outflows in Underground Hydrology (Hydrologischer Transport der radioaktiven Ausströmungen im unterirdischen Bereich)) geschaffen.

Die einfachste Version dieser Familie, das Programm TROUGH-1D, wurde mehrmals weiterentwickelt und ausgetestet, um den verschiedenen Teilaspekten der Arbeit von NAGRA gerecht zu werden.

Der vorliegende Bericht enthält eine technische Beschreibung und das Benutzerhandbuch für den Code.

R E S U M E

En vue de l'analyse de sécurité du dépôt final pour déchets nucléaires, on a créé un groupe de programmes pour ordinateur, appelé TROUGH (Transport of Radioactive Outflows in Underground Hydrology (Transport hydrologique des écoulements radioactifs dans le sous-sol)).

La version la plus simple de ce groupe, le programme TROUGH-1D, a été mise au point et testée plusieurs fois, afin de satisfaire les divers aspects partiels du travail de la Cédra.

Le présent rapport renferme une description technique et le manuel d'utilisation pour le code.

L I S T O F C O N T E N T S

	<u>Page</u>
1. INTRODUCTION	1
2. THEORETICAL MODEL	3
2.1 Transport in Groundwater	3
2.2 Matrix Diffusion	7
2.3 Saturation, Precipitation and Dissolution	9
2.4 Alternative Types of Nuclide Source	11
2.5 Boundary Conditions	14
3. THE FINITE DIFFERENCE EQUATIONS	15
3.1 General	15
3.2 Matrix Diffusion	19
3.3 Saturation, Precipitation and Dissolution	20
4. PROGRAM ORGANISATION	22
5. NOMENCLATURE LIST	25
6. BIBLIOGRAPHY	27
 <u>Appendix 1:</u> Input Data Description for TROUGH-1D	 28
<u>Appendix 2:</u> Sample problem and output	44

1. INTRODUCTION

TROUGH-1D is a general 1-dimensional finite difference code for the solution of the equations of transport of radionuclides in groundwater.

This document describes the mathematical problem to be solved and the numerical solution procedures used in the code. Special features incorporated in the code to handle particular problems are also described.

The general background to the problem of radionuclide transport in groundwater and the philosophy underlying the development of TROUGH is described in Reference 1.

Physically, the one-dimensional problem handled by TROUGH-1D represents a column of porous material through which groundwater is moving. The flow path may be truly 1-dimensional or purely radial in an axisymmetric (cylindrical) domain. In the latter case the migration path cross-section increases linearly with distance. The same formulation and coding have been used as in the MC.TRAD-2D code (see Ref. 2) to obtain this flexibility.

The radionuclide transport equation system describes the transport of nuclides released from a source into the groundwater over a period of time. A number of alternative ways are made available for modelling the source and for treating the mechanism of nuclide release to the transporting fluid.

Various processes may be treated by the calculations as follows:

- decay of the transported nuclides either in chains (non-branching) or singly.
- equilibrium or nonequilibrium sorption on solid surfaces in a conventional porous medium.
- diffusion into a solid matrix where an equivalent porous continuum models a fissured medium.

- saturation, precipitation and dissolution of all nuclides under locally constant element or nuclide specific saturation limits.

This latter feature enables, for instance, the calculation of the migration of a number of decay chains containing between them several nuclides of the same element which then compete for the total element solubility limit.

A range of inflow and outflow boundary conditions may be imposed on the modelled domain, permitting the simulation of a variety of physical situations.

Results are presented as spatial concentration distributions at selected times and as concentration or flux time histories at selected positions along the migration path. Inputs and outputs may be expressed in terms either of molal or activity concentration and flux.

Verification of the TROUGH-1D code has been undertaken within the framework of INTRACOIN (Ref. 3) with the exception of the matrix diffusion, which was verified using INTRACOIN level 1 and level 3 examples at a later date (Ref. 7). The cylindrical coordinate formulation is reported in Reference 2, where a detailed verification of MC.TRAD-2D is included.

2. THEORETICAL MODEL

2.1 Transport in Groundwater

Any scalar property, such as thermal energy or chemical concentration, is transported in a fluid by two principal mechanisms, convection and diffusion. A differential equation describing the transport process can be derived by considering the mass balance in an elemental cell using the following definitions:

Scalar property being transported = ϕ per kg of transporting fluid

Convective flux = $\rho U_i \phi$ per $m^2\text{-yr}$

Diffusive flux = $-D \frac{\partial \phi}{\partial x_i}$ per $m^2\text{-yr}$

where:

U is the specific fluid flux [$m^3 m^{-2} \text{ yr}^{-1}$]

D is the diffusivity [$m^2 \text{ yr}^{-1}$]

ρ is the density of the transporting fluid [$kg m^{-3}$]

i is the coordinate direction

In one dimension the time dependent form of this equation is:

$$\frac{\partial}{\partial t} (\rho \phi) = \frac{\partial}{\partial x} [\rho D \frac{\partial \phi}{\partial x}] - \frac{\partial}{\partial x} (\rho u \phi) + S_{x,t}^\phi \quad (2.1)$$

where $S_{x,t}^\phi$ is some source of ϕ per $m^3\text{-yr}$.

For groundwater migration problems one year is a reasonable time unit. However, the time scale of the model is fully determined by the input data and any appropriate unit may be used. It is only necessary that all input data values involving a time dimension are expressed in the same base unit.

In considering the transport of radionuclides in groundwater additional terms must be introduced into the above equations.

A first modification to equation 2.1 concerns the cross-sectional area of the flow path. Whether the groundwater is moving through a true porous material or a fissured, but otherwise impermeable, rock only a fraction of the total flowpath cross-section is available for fluid flow. This fraction is referred to as the porosity in either of the above cases and multiplies each term in equation 2.1.

Radioactive decay of the nuclide being transported, and the creation of new nuclides by decay of the parent in a decay chain can be introduced as particular components of the general source term, leaving the component $S_{x,t}^\phi$ to represent the injection of new material into the calculation domain.

Finally the effects of exchange of nuclides between the mobile component in the fluid and the immobile component adsorbed onto the surface of the solid must be considered.

Introducing these changes into equation 2.1, and writing the equation in terms of molar concentrations leads to the following expression:

$$\begin{aligned} \frac{\partial}{\partial t} (\varepsilon \rho N_1) + \frac{\partial}{\partial t} [(1-\varepsilon) \rho_s N_s] &= \frac{\partial}{\partial x} [\varepsilon \rho D \frac{\partial N_1}{\partial x}] - \frac{\partial}{\partial x} (\varepsilon \rho u N_1) + S_{x,t}^N \\ &\quad - \lambda [\varepsilon \rho N_1^* + (1-\varepsilon) \rho_s N_s^*] + \lambda^* [\varepsilon \rho N_1^* + (1-\varepsilon) \rho_s N_s^*] \end{aligned} \quad (2.2)$$

where properties pertaining to the parent nuclide are indicated by * and,

- N_1 = Number of moles per kg fluid
- N_s = Number of moles per kg solid
- u = Hydraulic velocity [m yr^{-1}]
- ε = Porosity [-]
- λ = Decay constant [yr^{-1}]

$$\rho \quad = \text{Fluid density } [\text{kg m}^{-3}]$$

$$\rho_s \quad = \text{Solid density } [\text{kg m}^{-3}]$$

In view of the widely differing time scales of the chemical sorption process and transport in naturally flowing groundwater it is generally reasonable to assume chemical equilibrium at all times. The model often used for trace concentrations assumes a linear sorption isotherm and this is therefore included as standard in TROUGH. It implies that the ratio of N_s to ρN_1 can be defined by a constant K_d so that N_s can be eliminated from equation 2.2 as follows for each of the three groups of terms in which it appears:

$$\begin{aligned} \varepsilon \rho N_1 + (1-\varepsilon) \rho_s N_s &= \varepsilon \rho [1 + \frac{1-\varepsilon}{\varepsilon} \rho_s K_d] N_1 \\ &= \varepsilon \rho R N_1 \end{aligned} \quad (2.3a)$$

where R is termed the retention factor.

This substitution reduces equation 2.2 to the following form:

$$\frac{\partial}{\partial t} (\varepsilon \rho R N_1) = \frac{\partial}{\partial x} [\varepsilon \rho D \frac{\partial N_1}{\partial x}] - \frac{\partial}{\partial x} (\varepsilon \rho u N_1) + s_{x,t} - \lambda \varepsilon \rho R N_1 + \lambda^* \varepsilon \rho R^* N_1^* \quad (2.3b)$$

There are certain cases, particularly during the evaluation of laboratory or limited-scale field experiments designed to check the mechanisms of migration, when the assumption of chemical equilibrium will be invalid. In practice, the domination of kinetic effects is most often felt in situations of higher flow rates or in problems of shorter time scale (viz. groundwater contamination during mining activities). Let us assume a mass transfer rate between fluid and solid surface of the form:

$$\dot{q}'' = k [(R-1) \varepsilon \rho N_1 - (1-\varepsilon) \rho_s N_s] \quad (2.4)$$

where \dot{q}'' is the net specific flux of nuclides from liquid to solid.

Implicit in this formulation are two assumptions:

- A single reaction rate constant, k may be defined
- the equilibrium situation may be described as in equation 2.3a, above.

We are no longer able to use the convenient combination technique. Instead, separate equations for the solid and liquid concentrations must be solved simultaneously.

$$\frac{\partial}{\partial t} (\varepsilon \rho N_1) = \frac{\partial}{\partial x} [\varepsilon \rho D \frac{\partial N_1}{\partial x}] - \frac{\partial}{\partial x} (\varepsilon \rho u N_1) - \lambda \varepsilon \rho N_1 + \lambda^* \varepsilon \rho N_1^* + S_1^N - \sigma k \{ (R-1) \varepsilon \rho N_1 - (1-\varepsilon) \rho_s N_s \} \quad (2.5a)$$

$$\frac{\partial}{\partial t} [(1-\varepsilon) \rho_s N_s] = \lambda^* (1-\varepsilon) \rho_s N_s^* - \lambda (1-\varepsilon) \rho_s N_s + S_s^N + \sigma k [(R-1) \varepsilon \rho N_1 - (1-\varepsilon) \rho_s N_s] \quad (2.5b)$$

It is to be noted here that, since the sorption mechanisms act only in the surface molecular layers of the solid particles, the concentration is dependent upon their surface/volume ratio. This parameter does not appear explicitly in the equations, but the active specific surface area σ [m^2/m^3] appears, multiplied by k , the transfer rate constant.

The above equation development can also be carried out for transport in a radial direction. In such a case equation 2.3b, for example, takes the form:

$$\frac{\partial}{\partial t} (\varepsilon \rho R N_1) = \frac{1}{r} \frac{\partial}{\partial r} \left(\varepsilon \rho D_r \frac{\partial N_1}{\partial r} \right) - \frac{1}{r} \frac{\partial}{\partial r} (\varepsilon \rho u r N_1) + S_{r,t} - \lambda \varepsilon \rho R N_1 + \lambda^* \varepsilon \rho R^* N_1^* \quad (2.6)$$

It will be noted that, apart from the change in the symbol for the independent space variable, the only alteration to the equation is in the diffusive term. A similar modification must be made to the corresponding term in equation (2.5a).

These transport equations are solved in TROUGH using a finite difference technique described in the next chapter.

2.2 Matrix Diffusion

A feature has been introduced into this particular version of TROUGH-1D which, for the transport of chemical species and nuclides, renders it capable of treating a fissured medium as an equivalent porous continuum. This is achieved by considering the solid component of the permeable medium as large blocks which can neither chemically nor thermally be in equilibrium with the flowing fluid component. The process treated is diffusion within the solid blocks. In the case of chemical diffusion, the process takes place along the microfissures of the solid. References 4 and 5 give an idea of the potential importance of this mechanism in the migration process.

The method has been described in detail in two publications (Refs. 7, 8), and requires only summarizing here. The blocks of solid material, which are surrounded by fissures carrying a flowing fluid, are modelled as slabs or spheres of appropriate size and quantity (fractional spheres, for instance are also allowed). These simple shapes permit an analytical one-dimensional solution to the diffusion problem in the solid. The analytical solution is embedded into the general finite difference solution to supply a source/sink term in the radionuclide transport equation (2.2).

The equation solved within the solid is the diffusion equation written (here for the general scalar ϕ) in the form:

$$\frac{\partial^2 \phi}{\partial \xi^2} - \frac{1}{\Gamma} \frac{\partial \phi}{\partial t} = \frac{\lambda}{\Gamma} \phi - \frac{\mu}{\Gamma} \quad (2.7)$$

whereby, at the beginning of each time step (whose length is determined by the requirements of the solution to (2.2)) the concentration profile is fitted to a function of the form:

$$f(\xi) = a_0 + \sum_{k=1}^m a_k \cosh\left(\frac{hk\xi}{l}\right) + b_k \cos\left(\frac{\pi k \xi}{2l}\right) \quad (2.8)$$

It should be noted here that Γ is the apparent diffusion coefficient in the matrix. If equilibrium sorption occurs on the surfaces of the microfissures, the retention effect is included in Γ and μ .

During the time step the time-varying concentration in the flowing fluid at the surface of the block ($\xi = \pm 1$) is idealised as a linear ramp function giving initial and boundary conditions:

$$\left. \begin{array}{l} \phi = f(\xi) \quad \text{for } t = 0 \\ \phi = \phi_0 + at \quad \text{for } 0 < t < \Delta t, \xi = \pm 1 \end{array} \right\} \quad (2.9)$$

A solution to equation 2.7 with boundary conditions 2.9 has been developed using extensions of standard solutions described by Carslaw & Jaeger (Ref. 6).

The analytical solution yields, at the end of the time step, the concentration distribution across the solid block. The flux of radionuclides across the fluid/solid interface at the block surface at any instant is given by the product of the local gradient of the concentration distribution and the effective diffusivity. This flux appears as a source term in the transport equation (2.2).

To avoid confusion the cumbersome algebraic expressions for this source, consisting of infinite series, are not included here. The expressions and details of their derivation may be found in Refs. 7 and 8.

The final expression for the source term can be summarised as follows:

$$S_M^\phi = - \Gamma \sigma_P \sum_{n=0}^{\infty} (\alpha I'_t + I'_t + I'_z) \quad (2.10)$$

where I'_t , I'_t and I'_z are appropriate groupings of the space and time integrals resulting from the solution.

By choice of the number of terms in the function 2.8 and of the number of points across the half-width (or radius) of the solid at which the function is fitted to the resulting distribution in readiness for the next time step, the accuracy of the solution may be influenced. The fitting procedure ensures conservation of the amount of nuclide ϕ during the timestep.

The retention factor for a fissured medium must be defined in a manner different from that for a porous medium. However, the form of the transport equation for one-dimensional fissure flow remains the same as (2.3b) or (2.5). All that is required is to define appropriate values for porosity, specific surface and retention factor.

A typical situation might be the analysis of migration through a single fissure on whose surface direct sorption is negligible in comparison with the diffusion in the microfissures in the neighbouring solid. In this case the retention factor is unity and the transport equation reduces to a simplified version of (2.3b).

$$\frac{\partial}{\partial t} (\varepsilon \rho N) + \frac{\partial}{\partial x} (\varepsilon \rho u N) = \frac{\partial}{\partial x} (\varepsilon \rho D_{xx} \frac{\partial N}{\partial x}) - \lambda \varepsilon \rho N + \lambda^* \varepsilon \rho N^* + S_M^N \quad (2.11)$$

2.3 Saturation, Precipitation and Dissolution

This version of TROUGH-1D includes the capability of treating problems in which the solubility of nuclides in the fluid is limited.

In such cases the calculated concentrations will be subject to an additional constraint in that they may not exceed the saturation value. Where there is a tendency for concentration to rise above this limit nuclides will be precipitated at a rate sufficient to exactly balance this tendency.

The concentration in fluid in contact with precipitate will remain at the solubility limit. Therefore, when at some later time the concentration is tending to decrease the precipitated nuclides may re-enter solution. Precipitated material is, of course, subject to the decay process, daughter nuclides being released (initially) into the fluid.

The rate of transfer of nuclides between a state of saturation in the fluid and the precipitate phase is modelled as a component of the source term in the transport equation (2.2):

$$\dot{q}''' = \epsilon \rho k_p (N_{sat} - N_l) \quad (2.12)$$

where:

k_p is a mass transfer rate coefficient (in yr^{-1})
 N_{sat} is the local saturation level of the nuclide in the liquid.

It will be observed that this kinetic formulation allows a treatment of the exchange between fluid and precipitate in a manner similar to that employed for the non-equilibrium sorption reaction.

A consequence of such a formulation is that a slow mass transfer rate may give rise to concentrations in the fluid significantly above the solubility limit during precipitation (or below it during dissolution).

A special problem occurs in the case of elements which appear in more than one isotopic form in a group of nuclides.

The concentration of each isotope in the fluid may be summed to give the total elemental concentration, and it is this latter value which is subject to the solubility limitation. By assuming that all isotopes of a single element behave similarly we can define an apparent isotopic solubility limit:

$$C_{sat,i} = \frac{M_{l,i} + M_{p,i}}{\sum_e (M_{l,i} + M_{p,i})} \cdot C_{sat,e} \quad (2.13)$$

where:

$M_{l,i}$ = number of moles of isotope i in solution
 $M_{p,i}$ = number of moles of isotope i in precipitate
 $C_{sat,e}$ = element solubility limit

$C_{sat,i}$ = isotope solubility limit
 Σ_e = signifies summation over all relevant isotopes of element e

The elemental solubility limits are assumed to be constant for each material zone. However, differing decay rates and source rates will result in isotopic solubility limits generally changing with time.

2.4 Alternative Types of Nuclide Source

Nuclides enter the modelled domain in one of the following ways:

- by diffusion and convection from a prescribed concentration at the upstream boundary,
- by injection of nuclides at some point along the migration path,
- by injection of contaminated water at some point in the migration path with consequent changes to the flow pattern.

Within these three modellable situations, three further options have been provided. The first of these is the specification of a leach rate from the initial mass of radioactive material present. In this case, the mass removal rate may be a constant, or may follow an arbitrary function of time. The decrement of the initial nuclide inventory is calculated according to:

$$\frac{\partial I_i}{\partial t} = \lambda^* I_i^* - \lambda I_i - \dot{m}_r \frac{I_i}{M_i} \quad (2.14)$$

where:

\dot{m}_r the instantaneous total mass removal rate $[kg yr^{-1}]$
 M_i the remaining material mass at time t $[kg]$
 I_i the amount of the nuclide remaining at t [moles]

Thus, the rate of release to the leaching fluid is given by the last term in (2.13):

$$f_r = \dot{m}_r \frac{I_i}{M_i} \quad [\text{moles yr}^{-1}] \quad (2.15)$$

In the particular case when \dot{m}_r is constant, the source material (a mixture of inert and active materials) is removed uniformly over a period:

$$t_r = \frac{M_i |_{t=0}}{\dot{m}_r} \quad (2.16)$$

At this point it is useful to introduce the variable, J , which is defined as the hypothetical inventory level at time t , given by the Bateman equations, rather than by equations like (2.14):

$$\frac{\partial J}{\partial t} = \lambda * J^* - \lambda J \quad (2.17)$$

whereby the mass removal by leaching or dissolution is not considered.

The relationship between J and I_i is:

$$J = I_i \left(1 + \frac{\int_0^t \dot{m}_r dt}{M_i} \right) \quad (2.18)$$

so that (2.15) becomes:

$$f_r = \frac{J}{t_r} \quad (2.19)$$

When \dot{m}_r is some general function of time the expression for f_r becomes somewhat more complicated. At present the code allows the specific mass release rate (i.e. as a fraction of the initial mass) to be described by a polynomial in time of up to order 4, so that (2.19) is replaced by:

$$\dot{I}_r = \sum_{k=0}^4 a_k t^k \cdot J \quad (2.20)$$

The mean rate of nuclide release during a time step is calculated so as to maintain an exact mass consistency:

$$\bar{I}_r = \frac{1}{\Delta t} \int_t^{t+\Delta t} I_r \cdot dt \quad (2.21)$$

The value of \bar{I}_r is either inserted directly as a source term at the point of injection, or divided by the injected water flux to give the nuclide concentration in the contaminated inflow (N_r).

A special option, introduced to meet the benchmark problem specifications of the INTRACOIN code comparison study, enables the contaminated inflow concentration to be applied as a boundary concentration, $N(0,t)$. However, since the concentration is determined on the basis of a purely convective inflow, the diffusive flux across the boundary introduces a small mass inconsistency between the inventory model and the migration model and this option is therefore not recommended for general use.

The second approach is the definition of the upstream boundary concentration or the nuclide injection rate, into either the transporting fluid or the contaminated water inflow, via an algebraic function of time fitted to data. The variables:

$N(0,t)$ or \dot{I}_r

(whichever is being used), or their logarithmus (to base 10) may be expressed as polynomials in time or \log_{10} (time) of up to order 4, (see Appendix I - Input Description). Here too an exact time step average of the polynomial is calculated.

Finally, the time history of the injection rate or the boundary concentration, calculated from a separate model or measured experimentally, may be supplied as input data.

2.5 Boundary Conditions

In order to calculate a solution of the finite difference equations it is essential that either the nuclide flux or the value of the concentration is specified at each end of the modelled domain. However, in modelling real situations it is not always possible to explicitly define boundary values. The following simple conceptual models of boundary behaviour have, therefore, been included in the code.

- Specified Boundary Concentrations

The use of this as an inflow (left-hand end) boundary condition has already been considered. Inflow and outflow boundary concentrations may also be set to zero, simulating contact with an infinite, well-mixed sink. Nuclides may cross the domain boundaries by both convection and diffusion.

- Zero Flux Boundary

Nuclides are unable to enter or leave the domain across one or both boundaries. This condition arises automatically in cylindrical geometry at $r = 0$.

- Convective Flux (Free Flow) Boundary

Fluid enters the domain with zero concentration or leaves with the local concentration, and there is no diffusive flux across the boundary. Similar exchanges of fluid between the modelled migration path and the surroundings can occur at discrete points within the domain.

- Resistive Exit Boundary

Nuclides leave the domain at the right-hand boundary to a zero concentration background. However, there is a constant mass transfer resistance at the boundary of the domain.

3. THE FINITE DIFFERENCE EQUATIONS

3.1 General

The transport equations presented in the previous section are solved in TROUGH by a finite difference technique. Figure 3-1 shows a section of the discretised calculation field and illustrates the nomenclature used in the computer code. Scalar properties (N_1 and N_s for each nuclide in a decay chain) are defined at each grid node while velocities are defined at the boundaries between the nodes. It should be noted that in general, i.e. for an irregular grid, calculation cell boundaries will not lie mid-way between grid nodes.

In writing the differential equations in a discretised form, it is assumed that the dependent variables change linearly between calculation nodes, while properties (e.g. ϵ , ρ , D) are constant in a control volume defined by the cell boundaries.

The subscripts P, E, W are used to denote a particular control volume and its east and west neighbours. Lower case subscripts denote values at the appropriate cell boundary while the superscript o indicates an old value (in the time sense).

Using this naming convention equation 2.3 can be re-written as follows (where ϕ represents the nuclide concentration N_1):

$$\begin{aligned} \frac{(\epsilon\rho R)_P}{\Delta t} [\phi_P - \phi_P^o] &= \frac{1}{\Delta x_P} \left\{ \frac{(\epsilon\rho D)_E}{\delta x_E} [\phi_E - \phi_P] - \frac{(\epsilon\rho D)_W}{\delta x_W} [\phi_P - \phi_W] \right\} \\ &\quad - \frac{1}{\Delta x_P} \left((\epsilon\rho U)_E \phi_E - (\epsilon\rho U)_W \phi_W \right) \\ &\quad - \lambda (\epsilon\rho R)_P \phi_P + \lambda^* (\epsilon\rho R^*)_P \phi_P^* + S_P \end{aligned} \quad (3.1)$$

In order to maintain flux continuity at the cell boundary it is necessary to define the diffusive coefficient term $(\epsilon\rho D)$ at the boundary (e

or w) as the harmonic mean of the coefficient value for the two adjacent cells. Thus for example:

$$(\varepsilon\rho D)_e = \frac{2\delta x_e (\varepsilon\rho D)_E (\varepsilon\rho D)_P}{\Delta x_E (\varepsilon\rho D)_P + \Delta x_P (\varepsilon\rho D)_E} \quad (3.2)$$

The values of ϕ at the cell boundaries are a weighted mean of the adjacent nodal values (a consequence of the assumed linear variation between nodes) for example,

$$\phi_e = \frac{1}{2} \frac{\Delta x_P}{\delta x_e} \phi_E + \frac{1}{2} \frac{\Delta x_E}{\delta x_e} \phi_P \quad (3.3)$$

In order to improve the stability of the algebraic solution scheme the general source term is expressed as a linear function of the transported variable, thus:

$$S^\phi = S_i^\phi + S_d^\phi \phi \quad (3.4)$$

if the source term is strongly non-linear the coefficients S_i and S_d must be continually updated in an iterative calculation. However, such a situation does not arise in the present application.

Introducing the definitions for ϕ_e and ϕ_w into equation 3.1 and rearranging yields, eventually an equation of the form:

$$[A_E + A_W + A_O - S_d] \phi_P = A_E \phi_E + A_W \phi_W + A_O \phi_P^O + S_i \quad (3.5)$$

where:

$$A_E = \frac{1}{\Delta x_P} \left\{ \frac{(\varepsilon\rho D)_e}{\delta x_e} - \frac{1}{2} \frac{\Delta x_P}{\delta x_e} (\varepsilon\rho U)_e \right\}$$

$$A_W = \frac{1}{\Delta x_P} \left\{ \frac{(\varepsilon\rho D)_w}{\delta x_w} + \frac{1}{2} \frac{\Delta x_P}{\delta x_w} (\varepsilon\rho U)_w \right\}$$

$$A_o = \frac{(\varepsilon \rho R)_P}{\Delta t}$$

$$S_i = \lambda^* (\varepsilon \rho R^*)_P \phi_P^* + S_P^\phi$$

$$S_d = - \lambda (\varepsilon \rho R)_P$$

An equation of this type can be written for each cell. With the values of ϕ specified at the ends of the calculation zone the set of (NI-2) equations can be solved simultaneously for the (NI-2) unknown values of ϕ giving a fully implicit solution of the differential equation.

In cylindrical geometry some of the expressions take on a slightly different form.

The mean diffusive coefficient between two nodes becomes, for example:

$$(\varepsilon \rho D)_e = \frac{(\varepsilon \rho D)_E (\varepsilon \rho D)_P \ln(r_E/r_P)}{(\varepsilon \rho D)_P \ln(r_E/r_e) + (\varepsilon \rho D)_E \ln(r_e/r_p)} \quad (3.6)$$

The A_E and A_W coefficients of equation (3.5) also change:

$$A_E = \frac{1}{\Delta r_P} \left(\frac{(\varepsilon \rho D)_e}{r_p \ln(r_E/r_P)} - \frac{1}{2} \frac{\Delta r_p}{\delta r_e} (\varepsilon \rho U)_e \right)$$

$$A_W = \frac{1}{\Delta r_P} \left(\frac{(\varepsilon \rho D)_w}{r_p \ln(r_p/r_w)} + \frac{1}{2} \frac{\Delta r_p}{\delta r_w} (\varepsilon \rho U)_w \right) \quad (3.7)$$

Since the path cross-section is a function of radius, it becomes essential to define the coordinate of the left hand boundary:

$$r_1 (\equiv x_1) \geq 0$$

For linear, one-dimensional problems with fixed boundary values a solution to the system of equations is obtained in one step. However, when the boundary conditions are expressed in terms of nuclide fluxes it becomes necessary to iterate, re-setting the boundary values after each iteration until the solution converges.

Alternatively, the equations of the form 3.5 could be solved individually for each ϕ_P using the values of ϕ_E and ϕ_W at the beginning of the time step. This explicit solution, while clearly much simpler to obtain than the implicit one, will become unstable unless the time steps are very small.

For the non-equilibrium problem a similar discretisation and re-arrangement of equation 2.5a leads to an equation identical in form to 3.6, but with the following amended coefficient definitions

$$A_O = \frac{(\varepsilon\rho)_P}{\Delta t}$$

$$S_i = \lambda * \varepsilon \rho N_i^* + S_1 + \sigma k(1-\varepsilon) \psi_P \quad (3.8)$$

$$S_d = -\lambda \varepsilon \rho - \sigma k(R-1) \varepsilon \rho$$

where ψ_P represents the solid concentration per m^3 in cell P ($\psi = \rho_s N_s$).

Equation 2.5b can also be written in a discretised form:

$$[A_O^S - S_d^S] \psi_P = S_i^S + S_d^L \phi_P \quad (3.9)$$

where:

$$A_O^S = \frac{(1-\varepsilon)}{\Delta t}$$

$$S_d^S = -\lambda(1-\varepsilon) - \sigma k(1-\varepsilon)$$

$$Si^S = \lambda * (1-\varepsilon) \psi_P^* + A_O^S \psi_P^O$$

$$Sd^1 = \sigma k (R-1) \varepsilon \rho$$

Rearranging equation 3.9 leads to an expression for ψ_P in terms of ϕ_P :

$$\psi_P = Si^\psi + Sd^\psi \phi_P \quad (3.10)$$

where:

$$Si^\psi = Si^S / (A_O^S - Sd^S)$$

$$Sd^\psi = Sd^1 / (A_O^S - Sd^S)$$

This expression can now be used to eliminate ψ_P from the coefficient definition 3.8, placing the Si^ψ part in the Si coefficient and the Sd^ψ part of the Sd coefficient. The set of equations 3.6 can now be solved as for the equilibrium case and the ψ_P values subsequently determined using equation 3.9.

3.2 Matrix Diffusion

The solution to the matrix diffusion equation, (2.10), can be rewritten as a source term in the above equations (part of S_P^ϕ) in terms of the liquid concentration ϕ_P by substituting for α as follows:

$$\alpha = (\phi_P - \phi_P^O) / \Delta t$$

Hence:

$$S_M^\phi = - \Gamma \sigma_P \sum_{n=0}^{\infty} \left(\frac{(\phi_P - \phi_P^O)}{\Delta t} I_t + I'_t + I_z \right) \quad (3.11)$$

which rearranges into the Si^M , Sd^M form:

$$S_M^\phi = Si^M + Sd^M \phi_P \quad (3.12)$$

where:

$$Si^M = - \Gamma \sigma_P \sum_{n=0}^{\infty} \left(I_t' - I_t \frac{\phi_P^0}{\Delta t} + I_z \right)$$

$$Sd^M = - \frac{\Gamma \sigma_P}{\Delta t} \sum_{n=0}^{\infty} I_t$$

Thus, the matrix diffusion effect appears as another specific component of the general source term and is included in the implicit calculation of the distribution of concentration in the groundwater.

3.3 Saturation, Precipitation and Distribution

The precipitation process described by equation 2.12 falls quite naturally into the linearised source term form. However, the relevant source coefficients may only be introduced after a preliminary solution has identified points in the domain where precipitation may occur. Once precipitation has been initiated in a calculation cell the quantity of precipitate must be monitored until it has all re-dissolved or decayed. Decaying precipitate appears as a supplementary source term in the daughter nuclide equation.

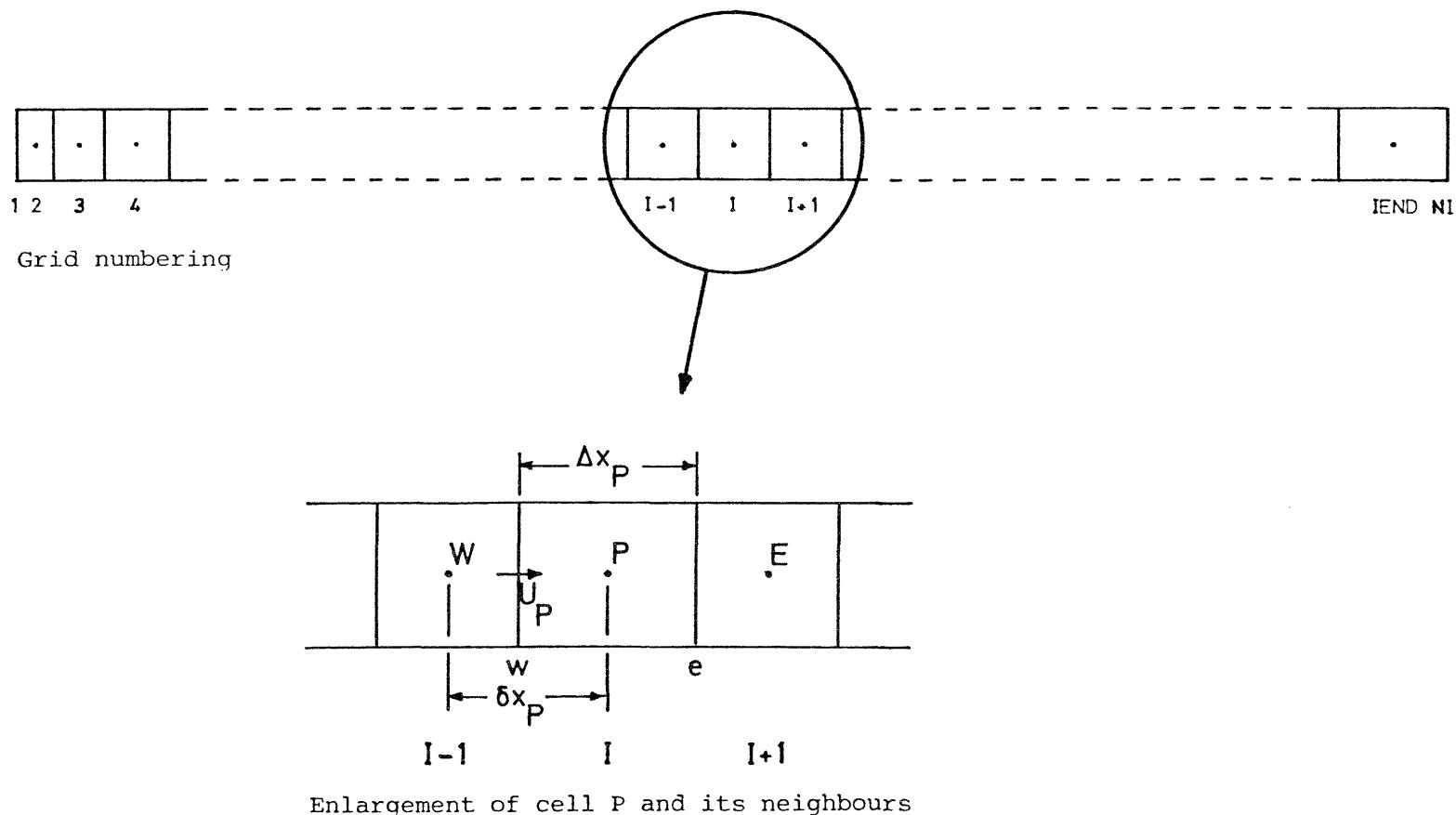


Figure 3-1: Nomenclature of the finite difference grid

4. PROGRAM ORGANISATION

Each time step of the calculation requires a solution of the finite difference equations (3.4) for each nuclide in the chain. The construction and solution of these equations takes place in a sequence of steps, each handled by a separate sub-routine called directly or indirectly from the main program routine. In addition, general input and output routines are provided and an unformatted binary restart file offers the facility of making time dependent calculations in a series of separate runs.

Data and results are transferred to and from the program via "logical tapes". These are permanent files which are referenced internally by the program using only their I/O unit number. The user must supply these files via the job control commands.

A description of the functions performed by each of the subroutines and subroutine entries is presented below:

PDRIVE A special sub-driver routine used during the precipitation calculation.

READIN Reads all input data from TAPE5.

ENTRY GET Reads restart file from TAPE 1.

INPUT Initialises arrays and program variables.

OUTPUT Writes spatial distribution of concentration in the groundwater at the end of the time step to TAPE6.

ENTRY CNHIST Writes time history of liquid (and solid if required) concentrations at reference locations to TAPE3.

ENTRY FLHIST Writes time history of nuclide fluxes at the left boundary of reference cells to TAPE4.

	ENTRY OUTITR	Writes iteration control values to TAPE6.
	ENTRY OUTPIT	Writes control values of the iterative precipitation calculation to TAPE6.
	ENTRY SAVE	Writes restart data to TAPE1.
PHYSIC		General physical data updating.
	ENTRY BOUND	Calculates nuclide inflows for the next time step (decaying inventory), or reads them from TAPE2.
	ENTRY SOURCE	Calculates source terms for nuclide annihilation (decay), creation (parent decay) and exchange between mobile and immobile components.
		Interprets nuclide inflows as concentrations or injection sources.
	ENTRY SOLIM	Calculates isotopic solubility limits.
	ENTRY PSOURC	Calculates source terms for nuclide precipitation or dissolution processes.
	ENTRY PSTOR	Calculates the quantity of precipitated nuclides.
	ENTRY FNFLUX	Calculates nuclide fluxes across cell boundaries.
	ENTRY FSSOLV	Calculates solid concentrations.
FDMODS		Explicit modifications to the finite difference equations.

	ENTRY OLDMOD	Transfers results to arrays labelled <u>Old</u> for use as initial conditions in next time step.
	ENTRY NEWMOD	Resets the calculated concentrations to the previous timestep values (used only if precipitation problem is treated).
	ENTRY PHIMOD	Modifies boundary values for next iteration.
SOLDIF		1st call calculates Si and Sd coefficients for Matrix Diffusion term in the finite difference equation. 2nd call calculates concentration distribution in the solid.
DISFIT		Fits a hyperbolic cosine series to the concentration distribution in the matrix.
	ENTRY SHIFT	Modifies the distribution function length scale for very slowly diffusing nuclides.
FDCOEF		Calculates A_E , A_W , Si, Sd coefficients for the finite difference equations.
SOLVER		Solves the set of simultaneous difference equations using a Gaussian Elimination method.

5. NOMENCLATURE LIST

A	Coefficient of the finite difference equation
a,b,c	Constants
C	Concentration of radionuclides in the micro-fissures [moles per m ³ of space]
D	Hydrodynamic dispersion coefficient [m ² /yr]
E,e	(subscripts) referring to specific neighbour locations in the finite difference grid (see figure 3-1)
h	Surface mass transfer rate coefficient [yr ⁻¹]
I	Inventory of a nuclide at any time [moles]
f _r	Rate of release of nuclides to the leaching fluid [mole/yr]
I'	A collection of terms following an integration
i	(subscript) referring to nuclide i
J	Instantaneous total inventory level [moles]
k	Sorption/desorption rate constant [m/yr]
K _d	Equilibrium concentration ratio ($N_s/\rho N_l$) [m ³ /kg]
k _p	Precipitation/dissolution rate constant [1/yr]
l	Depth of micro-fissure system [m]
l	(subscript) referring to liquid
M	Instantaneous total mass of inventory, precipitate or solute [kg]
m,n	Summation indices
m̄	Material mass flux (e.g. mass leaching rate) [kg/yr]
N	Atomic concentrations [moles/kg]
o	(subscript) referring to "old" values, i.e. values at the end of the previous time step in the numerical calculation
P	(subscript) referring to specific neighbour locations in the finite difference grid (see figure 3-1)
p	(subscript) referring to the precipitate
q"	Nuclide flux between solid and liquid [moles/(m ² yr)]
q'''	Nuclide flux between liquid and precipitate [moles/(m ³ yr)]
R	Retention factor $(1 + \frac{1-\epsilon}{\epsilon} \rho_s K_d)$ [-]
r	(subscript) referring to mass or nuclides being removed, or to leaching time
r _n	series term $[(2n+1)^2 \pi^2 \Gamma/41^2]$

S	General source term [moles/(yr m^3 of space)]
Si	Independent component of source term
Sd	Coefficient of dependent component of source term
s	(subscript) referring to solid
sat	(subscript) referring to the state of saturation
t	Time [yr]
u	Velocity of transporting fluid [m/yr]
w,w	(subscripts) referring to specific neighbour locations in the finite difference grid (see figure 3-1)
z	1-dimensional space coordinate in the microfissure system ($0 \leq z \leq 1$) [m]
α	Rate of change of concentration [moles/(m^3 yr)]
Γ	Effective diffusivity of microfissure system [m^2/yr]
ε	Porosity [-]
θ_n	Series term [$(2n+1)\pi/2l$]
λ	Decay constant [1/yr]
μ	Creation rate of nuclides by decay of parent [moles/(yr m^3 of solid)]
ρ	Density [kg/m^3]
σ	Sorbing surface area per m^3 of space [m^2/m^3]
ϕ	Concentration of radionuclides in liquid [moles/kg of liquid]
ψ	Concentration of radionuclides in solid [moles/ m^3 of solid]
X	Cross-sectional area of flowpath [m^2]

6. BIBLIOGRAPHY

- 1) Gilby D.J., Hopkirk R.J. - An integral approach to radionuclide transport modelling in fissured and porous media, NAGRA Technical Report NTB 83-13, Baden, Switzerland, 1984.
- 2) Hopkirk R.J., Gilby D.J. - MC.TRAD-2D: a computer program for modeling diffusive transport in rectangular or cylindrical two-dimensional coordinate systems, NAGRA Technical Report NTB 85-37, Baden, Switzerland, 1985.
- 3) Swedish Nuclear Power Inspectorate - INTRACOIN - International Nuclide Transport Code Intercomparison Study - Final Report level 1 - Code Verification, Stockholm, September 1984.
- 4) Neretnieks I. - Diffusion in the rock matrix - an important factor in radionuclide retardation, SKBF/KBS Teknisk Rapport 79-19, Stockholm, 1979.
- 5) Rasmusson A. and Neretnieks I. - Migration of radionuclides in fissured rock - the influence of micropore diffusion and longitudinal dispersion, SKBF/KBS Teknisk Rapport 80-24, Stockholm, December 1979.
- 6) Carslaw H.S. and Jaeger J.C. - Conduction of Heat in Solids, Oxford at the Clarendon Press, 1959.
- 7) Gilby D.J. and Hopkirk R.J. - A method for modelling the transport of nuclides in fissured rock with diffusion into the solid matrix, NAGRA technical report NTB83-06, Baden, Switzerland, 1983.
- 8) Hopkirk R.J. and Gilby D.J. - heat and mass transport in a domain containing both solid and fluid - an analytical model embedded in a numerical solution method, paper for presentation at 3rd International Conference on Numerical Methods in Thermal Problems, University of Washington, Seattle, USA, August 2nd - 5th, 1983.

A P P E N D I X 1

INPUT DATA DESCRIPTION FOR TROUGH-1D

A sample input listing is included at the end of this appendix in Table A1-1.

The input data is grouped into four blocks, as follows:

<u>BLOCK 1</u>	Specifies the general nature of the calculation
<u>BLOCK 2</u>	Specifies the time and space discretisation of the model
<u>BLOCK 3</u>	The physical parameters for the model
<u>BLOCK 4</u>	Specifies output tables
<u>BLOCK 5</u>	The injection/boundary/leaching source coefficients, where necessary

A line-by-line explanation of the individual items of data in each block is given here. This may be compared with Table A1-1, which contains the input necessary for running the case described in Appendix 2.

It is to be noted that the grid and variable arrays are dimensioned in this version to accommodate problems of the following size:

- up to 199 finite difference intervals along the migration path
- up to 24 transported chemical species in up to 4 separate chains,
each of maximum length 6
- up to 10 different material zones

BLOCK 1 - Type of Calculation

6 lines, alphanumeric and integer

Variables Input:

line 1	JTITLE	A80
line 2	NREST, NSTEPS, NITERS, NITP, NCHAIN	20I4
line 3	ISOURC, NPIC, LINLOG, INJECT, IENTRY, IEXIT,	
	INVENT, KOORD	20I4
line 4	ICHAIN, ISAT, ISDIFF, IEQUI	20I4
line 5	LCHAIN(4)	20I4
line(s) 6	LINK	20I4

Explanation:

JTITLE An 80 character job title, which is reproduced at the start of each output table.

NREST = 0 A new calculation

= 1 A restart calculation

= 2 Restart facility not used

NSTEPS Maximum number of time steps to be calculated

= 0 For steady state

NITERS Maximum number of iterations per time step (*)

NITP Maximum number of iterations of competitive solubility calculation.

NCHAIN 1-4 The number of separate decay chains to be considered

ISOURC An index specifying the nature of the nuclide source.

= 1:

The initial inventory is given by the STINV array for each nuclide. The mass leaching rate is constant during the leaching period and the nuclide source terms are calculated according to the Bateman equations.

= 2:

The initial inventory is given by the STINV array for each nuclide. The mass leaching rate is time-dependent, defined by the NPIC flag and the PNINV coefficients, thus:

$$\dot{m}_r = \sum_{K=1}^{NPIC} PNINV(I,K) * (TIME)^{K-1}$$

The nuclide source is calculated according to the Bateman equations and the instantaneous mass leaching rate.

= 3:

The individual nuclide release rates or boundary concentrations are time dependent, defined by the NPIC and LIN-LOG flags and the PNINV coefficients.

= 4:

The individual nuclide release rates or boundary concentrations are read from the time history contained on TAPE 2 (see BLOCK 5).

NPIC \leq 5 An index to define the number of polynomial coefficients, PNINV, to be read (see BLOCK 5).

When ISOURC = 1 or 4, NPIC is not used.

LINLOG An index to define the nature of the polynomial function when ISOURC = 3.

$$\begin{aligned}
 &= 1: \quad \text{linear } S = \sum_{k=0}^{NPIC-1} a_k t^k \\
 &= 2: \quad \text{log-linear } \log_{10}(S) = \sum_{k=0}^{NPIC-1} a_k t^k \\
 &= 3: \quad \text{log-log } \log_{10}(S) = \sum_{k=0}^{NPIC-1} a_k [\log_{10}(t)]^k
 \end{aligned}$$

where:

$$S = N_i(0, t) \text{ or } I_i(t)$$

a_k are the polynomial coefficients PNINV (nuclide, k+1) (see BLOCK 5).

INJECT The number of the calculation cell into which the nuclides are released (directly or indirectly).

If INJECT = 1 the nuclide release values are interpreted as inlet boundary concentrations.

IENTRY Inlet (left hand side) boundary condition index:

= -1 Zero nuclide flux

= 1 Specified boundary concentration $N_i(0, t)$ if INJECT = 1 and TIME < TIMOUT. FENTRY otherwise.

= 10 Convective inflow with boundary concentration and no diffusive boundary flux (free inflow).

IEXIT Outlet (right hand side) boundary condition index.

= -1 zero nuclide flux.

= 1 specified boundary concentration, FEXIT.

= 10 Convective outflow with last cell concentration and no diffusive boundary flux (free outflow).

= 20 Surface mass transfer resistance to background concentration FEXIT.

INVENT Concentrations and nuclide inventories according to the following table:

	Input	Time history outputs
= 1	activity	activity
= 2	moles	activity
= 3	activity	moles
= 4	moles	moles

Concentrations are expressed per litre of transporting fluid.

KOORD = 0 Linear transport in rectangular geometry.

= 1 Radial transport in cylindrical geometry.

ICHAIN = 0 Each of the nuclides is to be considered independently.

= 1 The nuclides form decay chains as described by LCHAIN.

ISAT	= 0	No precipitation treated
	= 1	Precipitation is to be treated
ISDIFF	= 0	No matrix diffusion treated
	= 1	Diffusion into solid slabs is to be treated
	= 2	Diffusion into solid spheres is to be treated
IEQUI	= 0	Equilibrium between solid and liquid exists at all times
	= 1	Non-equilibrium sorption case must be calculated
LCHAIN		The number of nuclides in each decay chain. For independent nuclides (i.e. ICHAIN = 0), the "chains" are simply convenient groupings of nuclides.
LINK		A 2-D array describing the shared solubility structure of the set of nuclides. The array consists of one row for each chain and one position in the row for each member of the chain. <u>Elements</u> which appear in more than one isotopic form are numbered sequentially and the element number is inserted in the LINK array in the appropriate position for each isotope. The positions for those nuclides, which are not subject to competitive solubility are filled with zeros.

* Note:

For fixed boundary concentrations (IENTRY = 1 and IEXIT = 1 or 20) a solution to the equation is obtained in a single sweep. NITERS may be put to = 1.

BLOCK 2 - Problem Discretisation

5 lines or sets of lines, various formats

Variables Input:

line 1	NI, NIPRINT	3I4
line 2	TIMAX, DT1, TIMCH, DT2, TIMOUT, TIMEX, TIME	7F8.0
line 3	XMIN, CROSS	7F8.0
line(s) 4	DX	free format
line(s) 5	NFLAG	free format

Explanation:

NI \leq 199	Number of calculation cells in the grid
NIPRINT	The number of the last cell in the migration path which is of interest and for which concentrations will be printed in the output of spatial distribution.
TIMAX	Time limit of calculation [yr]
DT1	Time step initially [yr]
TIMCH	Time at which time step size changes [yr]
DT2	Time step after TIMCH or maximum time step [yr]
TIMOUT *	Time at which concentration inflow stops [yr]
TIMEX	Expansion factor for time step size (effective only after TIMCH). If TIMEX = 0.0 time step size change directly to DT2 at TIMCH.
TIME	"Absolute time" at start of calculation [yr]. This must be > 0 if LINLOG = 2.

XMIN Coordinate of left-hand boundary of modelled domain. If XMIN > 0 in cylindrical geometry transport will be through an annular domain. [m].

CROSS Cross section of the flow path in rectangular geometry [m^2]. Fraction of full circle in cylindrical geometry.

DX Real array, length NI - Calculation cell widths [m]. First and last cell must be 0.0

NFLAG Integer array, length NI - flags indicating up to 10 different zones in the model. $1 \leq NFLAG \leq 10$.

* Note:

For ISOURC = 1 (uniform dissolution rate) TIMOUT is the total leach time.

for ISOURC = 2, TIMOUT is set internally to the TIME at which the time integral of the specific mass release rate function reaches 1. This value of total leach time is printed on the OUTPUT file.

for ISOURC > 2. The calculation or input of nuclide release values ceases at TIMOUT.

For ISOURC = 4 the nuclide release time history input dictates the time step size up to TIMOUT (see also BLOCK 5).

BLOCK 3 - Physical Data

19 lines or sets of lines

Variables Input:

line 1	THETA, ADIOS, CRIT	10F8.0
line 2	CINIT, CENTRY, CEXIT, HS	10F8.0
line 3	NLEAK, ILEAK	10I8
line 4	FLIN, FLEX	10F8.0
line 5	RNAME	5A8
line 6	ALAM	10F8.0
line 7	STINV	10F8.0
line 8	AKS	10F8.0
line 9	ADIS	10F8.0
line 10	EPS	10F8.0
line 11	DZ	10F8.0
line 12	ALZ	10F8.0
line 13	FISS	10F8.0
line 14	EMAT	10F8.0
line(s) 15	SOLD	10F8.0
line(s) 16	ARM	10F8.0
line(s) 17	AR	10F8.0
line(s) 18	AKM	10F8.0
line(s) 19	ASAT	10F8.0

Explanation:

THETA Weighting factor in the mixed differencing scheme:

- 1.0 fully implicit (recommended)
- 0.0 explicit
- 0.5 semi-implicit: Crank-Nicolson

ADIOS The calculation will be stopped if all the concentrations at the first reference point become less than ADIOS

CRIT The iteration process in the solution for a nuclide within a time step will be stopped when the normalised sum of the concentration changes in all cells between iterations (the field residual) falls below CRIT:

$$\sum_{2}^{NI-1} \frac{|DF|}{F} < CRIT$$

CINIT Concentration at model time zero [moles/l or activity/l].

CENTRY Concentration at inflow boundary.

CEXIT Concentration at outflow boundary (or background if IEXIT = 20).

HS Mass transfer coefficient at the right hand boundary of the domain [yr^{-1}]

NLEAK ≤ 9 Number of points at which transporting fluid enters or leaves the migration path, excluding the inflow and outflow boundaries.

ILEAK Array, length 9 - cell number at which transporting fluid enters or leaves the migration path.

FLIN Flux of transporting fluid entering the modelled domain at left-hand boundary [l/yr].

FLEX Array, length 9 - FLEX(K) = flux of transporting fluid exchanged with background in cell ILEAK(K) a positive value means an inflow to the modelled migration path [l/yr].

The following group of 4 lines is repeated once for each chain (max. 4 times).

RNAME Alphanumeric array, length 6 - the name of each nuclide.

ALAM Array, length 6 - Decay constant for each nuclide [yr⁻¹].

STINV Array, length 6 - Inventory of each nuclide at time zero
[moles or activity].

AKS Array, length 6 - precipitation/dissolution transfer
coefficient for each nuclide [1/yr]

ADIS Array, length 10 - Dispersivity constant in each material
zone [m²/yr]

EPS Array, length 10 - Flow path porosity in each zone [-]

DZ Array length 10 - Thickness of the migration path. Chan-
ges in DZ along the path are treated numerically as
changes in flowpath porosity.

The following block of 6 lines is required only if ISDIFF ≠ 0.

ALZ Array, length 10 - Mean slab half-thickness or sphere
radius in each zone [m].

FISS Array, length 10 - Specific surface of fissures in each
zone [m²/m³]

EMAT Array, length 10 - The porosity of the matrix in each
zone [-].

SOLD 2-D array, 10 columns, 1 row for each nuclide - Each row
contains the micro-fissure diffusivity for one nuclide in
each zone [m²/yr] *

ARM 2-D array, 10 columns, 1 row for each nuclide - Each row
contains the retention factors for one nuclide in the
matrix in each zone [-].

AR 2-D array, 10 columns, 1 row for each nuclide - Each row contains the retention factors for one nuclide in each zone [-]

The following array is only required if IEQUI \neq 0.

AKM 2-D array 10 columns, 1 row for each nuclide - Each row contains the value - Mass transfer coefficient \times interfacial area per m^3 - for one nuclide in each zone [1/yr]

The following array is only required if ISAT \neq 0.

ASAT 2-D array, 10 columns, 1 row for each nuclide - Each row contains the saturation concentration levels for one nuclide in each zone [moles/l of liquid].

* Note:

Diffusion takes place through the pore water trapped in the microfissures of the matrix. The molecular diffusivity of a nuclide in water may be multiplied by a factor to account for the tortuosity and constrictivity of the microfissure system yielding a pore diffusivity D_p . The value of this parameter is dependent on the material and the diffusing nuclide, although physically similar nuclides (e.g. heavy metal ions) tend to have the same D_p . It is this parameter which must be supplied as the data item SOLD.

Since diffusion occurs only in the pore water the effective diffusivity of the matrix is reduced to $\epsilon_M D_p$, where ϵ_M is the porosity of the matrix. During a transient process, sorption of the diffusing nuclide will affect the diffusive flux and result in an apparent diffusivity D_a ($= D_p / R$). It is generally this latter value which is measured in experimental studies since the very slow processes necessitate observations being made during the transient.

BLOCK 4 - Output Specification

2 lines, format 20I4

Variables Input:

line 1	NOJUMP, NIJUMP, ISKIP, JUMPD1,	20I4
	JUMPD2, NPJUMP, NOHIST	
line 2	NRTYP, ITYP	20I4

Explanation:

NOJUMP Jump factor for timestep output of concentration distribution. When NOJUMP = n, only timesteps 0, n, 2n, 3n, will be printed in file output.

NIJUMP Jump factor for iteration output.

ISKIP Jump factor for spatial concentration distribution printout at the end of each selected timestep.

JUMPD1 Jump factor for output of time histories up to the time TIMCH.

JUMPD2 As JUMPD1 for the period after TIMCH.

NPJUMP Jump factor for precipitation iteration output.

NOHIST = 0 No time histories will be created.

 = 1 Concentration time histories will be written to TAPE 3.

 = 2 Flux time histories will be written to TAPE 4.

 = 3 Both time histories will be written.

NRTYP Number of reference cells for which time histories of concentration or activity levels and fluxes will be generated (NRTYP \leq 10, but see Note B4.1)*

ITYP Integer array, length 10 - Index(es) of the reference cell(s).

If NRTYP = 2, IEQUI = 1 and ITYP(1) = ITYP(2): Liquid and solid concentrations will be written at the specified location.

It should be noted, in reference to Figure 3-1 of the main text of this manual, that the concentrations are computed for the nodes of the typical cells, but the fluxes refer to the nuclide flux into those cells across their left-hand boundaries.

* Note B4.1:

The product NRTYP * Number of nuclides should not be greater than 10 if tidy output tables are required. Where this condition cannot be observed it may be desirable to write a simple post-processor to meet user requirements for tabulated output. The format of the time history tables is (11E12.4). The first field contains the model time [yrs], and the format repeats as often as necessary.

BLOCK 5 - Nuclide Source Data

This block of data is only required if ISOURC > 1.

Variables Input:

line(s) 1	PNINV	5F10.0
line(s) 2	FORM	5A8

Explanation:

PNINV A 2-dimensional array of polynomial coefficients which are interpreted according to ISOURC, INJECT and LINLOG (see BLOCK 1).

If ISOURC = 2, NPIC coefficients are expected on one line.

If ISOURC = 3, NPIC coefficients for each nuclide are expected, one line per nuclide.

If ISOURC = 4, line(s) 1 must be omitted.

FORM A character array containing the FORTRAN specification of the format of the file TAPE 2. This file contains the time history of inflow concentration or injection rate for each nuclide.

When ISOURC = 4, the program reads one value of time followed by the boundary concentration or injection rate for each nuclide from TAPE 2 at each step. It is assumed that the nuclide data is the instantaneous value at the given time and that values have changed linearly since the previously input time point. The time history need extend only up to TIMOUT after which the normal time step procedure takes over.

*** SAMPLE PROBLEM ***

```

0 100 20 5 1
1 0 0 1 1 1 0
1 0 0 1
3
0 0 0
27 18
2.5E5 250.0 1.0E4 500. 1.0E4 0.0 0.0
0.0 100.0
0.0 10*25.0 15*50.0 0.0
11*1 16*2
1.0 1.0E-16 1.0E-5
0.0 0.0 0.0 0.0
0
1.0
CM-245 NP-237 U-233
8.16E-5 3.24E-7 4.35E-6
0.7 1.0 0.004
1.0E+10 1.0E+10 1.0E+10
50.0 50.0
0.01 0.02
1.00 1.00
500. 70.
100. 50.
60. 30.
1.0E-4 1.0E-4
2.0E-4 2.0E-4
2.5E-4 2.5E-4
20 999 2 4 2 1 3
2 16 16

```

```

JTITLE
NREST,NSTEPS,NITERS,NITF,NCHAIN
ISOURC,NFIC,LINLOG,INJECT,IENTRY,IEXIT,INVENT,KOOR
ICHAIN,ISAT,ISDIFF,IEQUI
LCHAIN(4)
LINK(1,6)
NI,NIFPRINT
TIMAX,DT1,TIMCH,DT2,TIMOUT,TIMEX,TIME
XMIN,CROSS

DX,NFLAG
THETA,AIIOS,CRIT
CINIT,CENTRY,CEXIT,HS
NLEAK,ILEAK(9)
FLIN,FLEX(9)
RNAME(1,6)
ALAM(1,6)
STINV(1,6)
AKS(1,6)
ADIS(10)
EPS(10)
IZ(10)
AR(10,1)
AR(10,2)
AR(10,3)
AKM(1,10)
AKM(2,10)
AKM(3,10)
NOJUMP,NIJUMP,ISKIP,JUMPD1,JUMPD2,NPJUMP,NOHIST
NRITYP,ITYP(10)

```

Table A1-1: Sample Input Data File

A P P E N D I X 2

Sample Problem and Output

The sample input data file presented in Table A1-1 describes a problem involving the transport of a three member nuclide chain through a two layer porous medium. In Table A2-1 the physical parameters of the situation being modelled are described for comparison with the input data file. Tables A2-2, A2-3 and A2-4 contain samples of the output generated. The first of these gives the spatial distributions of concentration at specified times, whilst the second and third are the time histories respectively of concentrations and fluxes for a "typical" cell. The cell selected is 475 m downstream from the point of injection of the radionuclides into the moving groundwater, so the time histories are for concentrations at the central nodal point and for the flux entering the left-hand-face of the cell.

In both of the time history output samples, the JUMPD1 and JUMPD2 flags have been set to give values every 1'000 years. Table A2-3 contains concentration time histories for both liquid and solid phases at the 475 m point. Table A2-4 includes the nuclide fluxes into the monitoring cell (at 450 m). Since for solid and liquid time histories the monitoring cell must be selected twice, the flux time histories are printed twice in this table.

Figure A2-1 shows a plot of the time history output file up to 40'000 years from which the consequences of the sorption/desorption mechanisms before and after the leaching can be clearly seen.

The radionuclides are assumed to be leached at a uniform rate from an initially prescribed inventory over a period of 10'000 years into a flow path with a cross-section of 100 m^2 and a groundwater through flow of $1 \text{ m}^3/\text{yr}$.

Non-equilibrium sorption reactions are considered between the moving groundwater and the porous solid.

Two important considerations in constructing numerically reliable models are illustrated by this sample problem.

In order to avoid numerical problems in mixed convection/diffusion calculations the finite difference cells must be dimensioned in accordance with the following rule:

$$\Delta x \leq \frac{1}{2} \frac{D}{u}$$

This gives a maximum cell size of 25 m in zone 1 and 50 m in zone 2.

Secondly, so as to minimise the effect of a possibly artificial exit boundary condition the calculation domain is extended some 500 m downstream from the monitoring point. With a well defined outflow boundary condition this domain modification would not be necessary.

Table A2-1 a)

Parameter	Symbol Units	Zone 1	Zone 2
Porosity	ϵ [-]	0.01	0.005
Velocity	u [m/yr]	1.00	0.50
Dispersivity	D [m^2/yr]	50	50
Length	[m]	250	250

Table A2-1 b)

Parameter	Symbol	Units	Nuclide 1 ^{245}Cm	Nuclide 2 ^{237}Np	Nuclide 3 ^{233}U
Initial Inventory	I	Activity (arbitrary)	0.7	1.0	0.004
Half-Life		[years]	8'500	2'140'000	159'200
Decay Constant	λ	[years ⁻¹]	8.155×10^{-5}	3.239×10^{-7}	4.354×10^{-6}
Mass Transfer Coefficient	α_k	[years ⁻¹]	1.0×10^{-4}	2.0×10^{-4}	2.5×10^{-4}
Retention Factor Zone 1	R	---	500	100	60
Retention Factor Zone 2	R	---	70	50	30

*** SAMPLE PROBLEM ***

STEP = 20 TIME = 5.000E+03 DT = 2.500E+02 CONCENTRATION DISTRIBUTION (MOLES/KG = MOLES/L)
ITER = 1 SSUM = 0. SATITER = 1 CONV = 0.

	I = 1	3	5	7	9	11	13	15	17
CM-245	5.76E-04	2.97E-04	1.24E-04	5.03E-05	2.02E-05	8.33E-06	4.50E-06	2.38E-06	1.25E-06
NF-237	3.79E-01	2.93E-01	2.04E-01	1.40E-01	9.39E-02	5.82E-02	3.00E-02	1.50E-02	7.35E-03
U-233	1.30E-04	1.59E-04	1.61E-04	1.44E-04	1.18E-04	8.86E-05	5.78E-05	3.56E-05	2.12E-05

X(M)= .00 37.50 87.50 137.50 187.50 237.50 325.00 425.00 525.00

STEP = 40 TIME = 1.000E+04 DT = 2.500E+02 CONCENTRATION DISTRIBUTION (MOLES/KG = MOLES/L)
ITER = 1 SSUM = 0. SATITER = 1 CONV = 0.

	I = 1	3	5	7	9	11	13	15	17
CM-245	3.83E-04	2.29E-04	1.11E-04	5.17E-05	2.33E-05	1.07E-05	6.19E-06	3.50E-06	1.96E-06
NF-237	4.27E-01	3.62E-01	2.83E-01	2.15E-01	1.59E-01	1.08E-01	6.35E-02	3.57E-02	1.96E-02
U-233	1.76E-04	2.98E-04	3.68E-04	3.74E-04	3.43E-04	2.85E-04	2.10E-04	1.45E-04	9.57E-05

X(M)= .00 37.50 87.50 137.50 187.50 237.50 325.00 425.00 525.00

STEP = 60 TIME = 1.975E+04 DT = 5.000E+02 CONCENTRATION DISTRIBUTION (MOLES/KG = MOLES/L)
ITER = 1 SSUM = 0. SATITER = 1 CONV = 0.

	I = 1	3	5	7	9	11	13	15	17
CM-245	0.	2.15E-05	2.35E-05	1.72E-05	1.07E-05	6.34E-06	4.27E-06	2.77E-06	1.76E-06
NF-237	0.	3.15E-02	6.24E-02	8.02E-02	8.59E-02	8.10E-02	6.75E-02	5.09E-02	3.59E-02
U-233	0.	1.51E-04	3.25E-04	4.53E-04	5.27E-04	5.48E-04	5.18E-04	4.43E-04	3.55E-04

X(M)= .00 37.50 87.50 137.50 187.50 237.50 325.00 425.00 525.00

STEP = 80 TIME = 2.975E+04 DT = 5.000E+02 CONCENTRATION DISTRIBUTION (MOLES/KG = MOLES/L)
ITER = 1 SSUM = 0. SATITER = 1 CONV = 0.

	I = 1	3	5	7	9	11	13	15	17
CM-245	0.	6.39E-06	8.71E-06	7.57E-06	5.48E-06	3.70E-06	2.70E-06	1.90E-06	1.31E-06
NF-237	0.	1.14E-02	2.83E-02	4.36E-02	5.50E-02	6.15E-02	6.21E-02	5.56E-02	4.59E-02
U-233	0.	8.01E-05	2.13E-04	3.51E-04	4.77E-04	5.85E-04	6.60E-04	6.63E-04	6.12E-04

X(M)= .00 37.50 87.50 137.50 187.50 237.50 325.00 425.00 525.00

STEP = 100 TIME = 3.975E+04 DT = 5.000E+02 CONCENTRATION DISTRIBUTION (MOLES/KG = MOLES/L)
ITER = 1 SSUM = 0. SATITER = 1 CONV = 0.

	I = 1	3	5	7	9	11	13	15	17
CM-245	0.	1.95E-06	3.17E-06	3.17E-06	2.59E-06	1.94E-06	1.51E-06	1.14E-06	8.30E-07
NF-237	0.	4.62E-03	1.34E-02	2.34E-02	3.35E-02	4.29E-02	5.01E-02	5.14E-02	4.78E-02
U-233	0.	4.07E-05	1.24E-04	2.31E-04	3.55E-04	4.97E-04	6.42E-04	7.30E-04	7.55E-04

X(M)= .00 37.50 87.50 137.50 187.50 237.50 325.00 425.00 525.00

Table A2-2: Spatial distributions of nuclide concentrations at selected timesteps
[atoms or moles / kg liquid]

*** SAMPLE PROBLEM ***

TIME	TIME HISTORIES OF THE ACTIVITY LEVEL			(ACTIVITY UNIT/LITRE IN LIQUID)			ACTIVITY UNIT/CU.M. IN SOLID)	
	475.0 M CM-245	475.0 M NP-237	475.0 M U-233	475.0 M CM-245	475.0 M NP-237	475.0 M U-233		
1.0000E+03	6.8028E-11	8.6461E-10	1.3387E-11	7.8721E-09	1.2848E-07	1.5468E-09		
2.0000E+03	8.6959E-11	1.3633E-09	2.7269E-11	1.6909E-08	3.1858E-07	4.8678E-09		
3.0000E+03	1.0557E-10	1.9520E-09	4.8778E-11	2.6889E-08	5.7555E-07	1.0726E-08		
4.0000E+03	1.2336E-10	2.6316E-09	7.9276E-11	3.7599E-08	9.0391E-07	1.9931E-08		
5.0000E+03	1.4105E-10	3.4024E-09	1.2004E-10	4.8839E-08	1.3075E-06	3.3298E-08		
6.0000E+03	1.5762E-10	4.2638E-09	1.7222E-10	6.0425E-08	1.7893E-06	5.1634E-08		
7.0000E+03	1.7326E-10	5.2149E-09	2.3688E-10	7.2182E-08	2.3518E-06	7.5723E-08		
8.0000E+03	1.8787E-10	6.2544E-09	3.1495E-10	8.3957E-08	2.9967E-06	1.0631E-07		
9.0000E+03	2.0139E-10	7.3803E-09	4.0723E-10	9.5607E-08	3.7252E-06	1.4409E-07		
1.0000E+04	2.1378E-10	8.5904E-09	5.1440E-10	1.0701E-07	4.5378E-06	1.8971E-07		
1.0750E+04	1.9425E-10	8.5252E-09	5.8554E-10	1.1271E-07	5.0786E-06	2.2783E-07		
1.1750E+04	1.9606E-10	9.2590E-09	7.0102E-10	1.1944E-07	5.8047E-06	2.8430E-07		
1.2750E+04	1.9684E-10	9.9644E-09	8.2249E-10	1.2521E-07	6.5307E-06	3.4657E-07		
1.3750E+04	1.9667E-10	1.0638E-08	9.4863E-10	1.3008E-07	7.2513E-06	4.1403E-07		
1.4750E+04	1.9566E-10	1.1279E-08	1.0781E-09	1.3406E-07	7.9615E-06	4.8601E-07		
1.5750E+04	1.9388E-10	1.1885E-08	1.2098E-09	1.3721E-07	8.6570E-06	5.6181E-07		
1.6750E+04	1.9144E-10	1.2454E-08	1.3426E-09	1.3956E-07	9.3340E-06	6.4072E-07		
1.7750E+04	1.8841E-10	1.2987E-08	1.4752E-09	1.4118E-07	9.9891E-06	7.2204E-07		
1.8750E+04	1.8486E-10	1.3481E-08	1.6069E-09	1.4210E-07	1.0620E-05	8.0505E-07		
1.9750E+04	1.8088E-10	1.3937E-08	1.7366E-09	1.4239E-07	1.1223E-05	8.8910E-07		
2.0750E+04	1.7652E-10	1.4356E-08	1.8637E-09	1.4209E-07	1.1797E-05	9.7354E-07		
2.1750E+04	1.7184E-10	1.4736E-08	1.9873E-09	1.4125E-07	1.2340E-05	1.0578E-06		
2.2750E+04	1.6692E-10	1.5079E-08	2.1069E-09	1.3994E-07	1.2851E-05	1.1412E-06		
2.3750E+04	1.6179E-10	1.5386E-08	2.2219E-09	1.3819E-07	1.3330E-05	1.2234E-06		
2.4750E+04	1.5650E-10	1.5657E-08	2.3319E-09	1.3606E-07	1.3774E-05	1.3038E-06		
2.5750E+04	1.5111E-10	1.5893E-08	2.4365E-09	1.3359E-07	1.4185E-05	1.3820E-06		
2.6750E+04	1.4564E-10	1.6094E-08	2.5354E-09	1.3083E-07	1.4561E-05	1.4577E-06		
2.7750E+04	1.4013E-10	1.6264E-08	2.6283E-09	1.2781E-07	1.4903E-05	1.5304E-06		
2.8750E+04	1.3462E-10	1.6401E-08	2.7151E-09	1.2458E-07	1.5211E-05	1.6001E-06		
2.9750E+04	1.2913E-10	1.6509E-08	2.7957E-09	1.2117E-07	1.5487E-05	1.6663E-06		
3.0750E+04	1.2369E-10	1.6587E-08	2.8699E-09	1.1762E-07	1.5729E-05	1.7289E-06		
3.1750E+04	1.1832E-10	1.6638E-08	2.9378E-09	1.1395E-07	1.5939E-05	1.7878E-06		
3.2750E+04	1.1303E-10	1.6663E-08	2.9993E-09	1.1020E-07	1.6119E-05	1.8428E-06		
3.3750E+04	1.0784E-10	1.6663E-08	3.0546E-09	1.0638E-07	1.6268E-05	1.8939E-06		
3.4750E+04	1.0277E-10	1.6640E-08	3.1036E-09	1.0254E-07	1.6388E-05	1.9410E-06		
3.5750E+04	9.7830E-11	1.6594E-08	3.1466E-09	9.8676E-08	1.6480E-05	1.9840E-06		
3.6750E+04	9.3024E-11	1.6528E-08	3.1837E-09	9.4820E-08	1.6545E-05	2.0230E-06		
3.7750E+04	8.8362E-11	1.6443E-08	3.2151E-09	9.0986E-08	1.6585E-05	2.0581E-06		
3.8750E+04	8.3850E-11	1.6339E-08	3.2408E-09	8.7190E-08	1.6600E-05	2.0892E-06		
3.9750E+04	7.9492E-11	1.6219E-08	3.2612E-09	8.3444E-08	1.6592E-05	2.1164E-06		

Table A2-3: Time history output of activity concentrations in both liquid and solid in the selected monitor cell
 [activity / m³ liquid]

*** SAMPLE PROBLEM ***

TIME	TIME HISTORIES OF THE TOTAL ACTIVITY FLUX ACROSS THE CELL BOUNDARIES (ACTIVITY UNIT/YEAR)					
	450.0 M CM-245	450.0 M NP-237	450.0 M U-233	450.0 M CM-245	450.0 M NP-237	450.0 M U-233
1.0000E+03	1.4296E-07	2.0479E-06	2.6616E-08	1.4296E-07	2.0479E-06	2.6616E-08
2.0000E+03	1.7813E-07	3.0806E-06	5.1495E-08	1.7813E-07	3.0806E-06	5.1495E-08
3.0000E+03	2.1191E-07	4.2556E-06	8.8867E-08	2.1191E-07	4.2556E-06	8.8867E-08
4.0000E+03	2.4403E-07	5.5685E-06	1.4031E-07	2.4403E-07	5.5685E-06	1.4031E-07
5.0000E+03	2.7425E-07	7.0139E-06	2.0715E-07	2.7425E-07	7.0139E-06	2.0715E-07
6.0000E+03	3.0240E-07	8.5859E-06	2.9049E-07	3.0240E-07	8.5859E-06	2.9049E-07
7.0000E+03	3.2836E-07	1.0278E-05	3.9120E-07	3.2836E-07	1.0278E-05	3.9120E-07
8.0000E+03	3.5204E-07	1.2084E-05	5.0993E-07	3.5204E-07	1.2084E-05	5.0993E-07
9.0000E+03	3.7340E-07	1.3995E-05	6.4712E-07	3.7340E-07	1.3995E-05	6.4712E-07
1.0000E+04	3.9241E-07	1.6006E-05	8.0301E-07	3.9241E-07	1.6006E-05	8.0301E-07
1.0750E+04	3.4578E-07	1.5106E-05	8.9257E-07	3.4578E-07	1.5106E-05	8.9257E-07
1.1750E+04	3.4488E-07	1.5990E-05	1.0464E-06	3.4488E-07	1.5990E-05	1.0464E-06
1.2750E+04	3.4235E-07	1.6793E-05	1.2024E-06	3.4235E-07	1.6793E-05	1.2024E-06
1.3750E+04	3.3839E-07	1.7516E-05	1.3584E-06	3.3839E-07	1.7516E-05	1.3584E-06
1.4750E+04	3.3319E-07	1.8161E-05	1.5128E-06	3.3319E-07	1.8161E-05	1.5128E-06
1.5750E+04	3.2692E-07	1.8729E-05	1.6640E-06	3.2692E-07	1.8729E-05	1.6640E-06
1.6750E+04	3.1973E-07	1.9222E-05	1.8107E-06	3.1973E-07	1.9222E-05	1.8107E-06
1.7750E+04	3.1178E-07	1.9644E-05	1.9517E-06	3.1178E-07	1.9644E-05	1.9517E-06
1.8750E+04	3.0319E-07	1.9996E-05	2.0862E-06	3.0319E-07	1.9996E-05	2.0862E-06
1.9750E+04	2.9410E-07	2.0284E-05	2.2134E-06	2.9410E-07	2.0284E-05	2.2134E-06
2.0750E+04	2.8460E-07	2.0508E-05	2.3326E-06	2.8460E-07	2.0508E-05	2.3326E-06
2.1750E+04	2.7481E-07	2.0674E-05	2.4435E-06	2.7481E-07	2.0674E-05	2.4435E-06
2.2750E+04	2.6481E-07	2.0784E-05	2.5457E-06	2.6481E-07	2.0784E-05	2.5457E-06
2.3750E+04	2.5468E-07	2.0842E-05	2.6390E-06	2.5468E-07	2.0842E-05	2.6390E-06
2.4750E+04	2.4450E-07	2.0852E-05	2.7234E-06	2.4450E-07	2.0852E-05	2.7234E-06
2.5750E+04	2.3432E-07	2.0816E-05	2.7988E-06	2.3432E-07	2.0816E-05	2.7988E-06
2.6750E+04	2.2420E-07	2.0738E-05	2.8653E-06	2.2420E-07	2.0738E-05	2.8653E-06
2.7750E+04	2.1420E-07	2.0622E-05	2.9231E-06	2.1420E-07	2.0622E-05	2.9231E-06
2.8750E+04	2.0434E-07	2.0471E-05	2.9725E-06	2.0434E-07	2.0471E-05	2.9725E-06
2.9750E+04	1.9467E-07	2.0287E-05	3.0135E-06	1.9467E-07	2.0287E-05	3.0135E-06
3.0750E+04	1.8521E-07	2.0075E-05	3.0466E-06	1.8521E-07	2.0075E-05	3.0466E-06
3.1750E+04	1.7599E-07	1.9835E-05	3.0721E-06	1.7599E-07	1.9835E-05	3.0721E-06
3.2750E+04	1.6704E-07	1.9573E-05	3.0904E-06	1.6704E-07	1.9573E-05	3.0904E-06
3.3750E+04	1.5836E-07	1.9289E-05	3.1017E-06	1.5836E-07	1.9289E-05	3.1017E-06
3.4750E+04	1.4997E-07	1.8986E-05	3.1066E-06	1.4997E-07	1.8986E-05	3.1066E-06
3.5750E+04	1.4188E-07	1.8667E-05	3.1053E-06	1.4188E-07	1.8667E-05	3.1053E-06
3.6750E+04	1.3409E-07	1.8334E-05	3.0983E-06	1.3409E-07	1.8334E-05	3.0983E-06
3.7750E+04	1.2660E-07	1.7988E-05	3.0860E-06	1.2660E-07	1.7988E-05	3.0860E-06
3.8750E+04	1.1943E-07	1.7632E-05	3.0687E-06	1.1943E-07	1.7632E-05	3.0687E-06
3.9750E+04	1.1256E-07	1.7268E-05	3.0469E-06	1.1256E-07	1.7268E-05	3.0469E-06
SUM FLUXES:	4.2633E-03	3.0857E-01	3.7698E-02	4.2633E-03	3.0857E-01	3.7698E-02
MAX FLUXES:	3.9241E-07	2.0852E-05	3.1066E-06	3.9241E-07	2.0852E-05	3.1066E-06

Table A2-4: Time history output of activity fluxes into the monitor cell. Note here the repetition of each time history due to the necessary double specification of monitor cell (for liquid plus solid concentrations). [activity / yr]

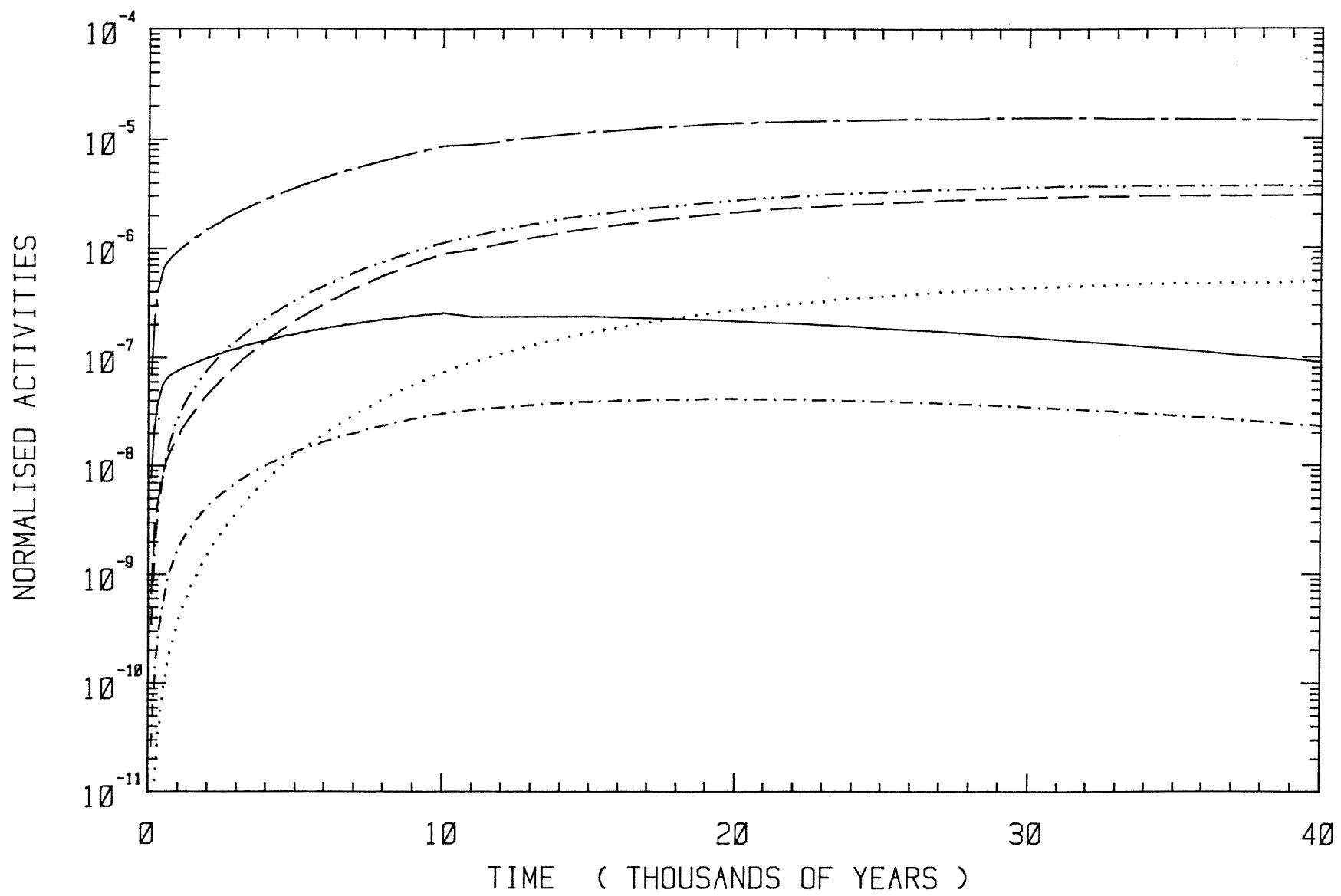


Figure A2-1:
ACTIVITY TIME HISTORIES AT MONITORING POINT