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FARF33 Version 1.1

User's Guide

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This report concerns a study which was conducted for SKB. The conclusions and viewpoints presented in the report are those of the authors. SKB may draw modified conclusions, based on additional literature sources and/or expert opinions.

A pdf version of this document can be downloaded from www.skb.se.

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1 Introduction

1.1 Background

The far-field code FARF33 calculates the transport of dissolved radionuclides through the fractured rock using a stream tube concept. It is based upon and is closely related to a previous far-field code called FARF31 that SKB developed for use with the probabilistic PROPER package. Both models are intended as tools to aid performance assessments of repositories for radioactive waste. Commonly, input data is taken from a groundwater model and a near-field model. The transport model includes advection and dispersion of a number of radionuclides along a streamline in fractured rock, with retention due to matrix diffusion and sorption taken into account. The model also includes chain decay. The solution method of FARF31 is based on analytical solution in the Laplace domain followed by numerical inversion of the Laplace transform and convolution with the input function to obtain the output function (Norman and Kjellbert 1990).

Unlike FARF31, the newer FARF33 additionally takes the effect of colloids into account when predicting migration rates of radionuclides in groundwater. It has been suggested that colloids can be important, and this has been studied by Cvetkovic (2003, 2004). A program called Collage II Plus has been studied and used as a starting point for this project. The model behind the Collage II Plus code is roughly equivalent with the FARF31 model, but it also includes transport equations for radionuclides sorbed onto colloids. It also has no option to include more than one nuclide in the simulation; hence chain decay cannot be simulated. The solution method of Collage II Plus is very similar to the FARF31 method, with analytic solution in the Laplace domain followed by numerical Laplace inversion.

It would probably be possible to extend the FARF31 solution scheme with a colloid phase in addition to the solute as long as only unidirectional transfer between the phases is allowed. However, for FARF33 another more general approach has been chosen instead. The transport equations, including both solute and colloid phases for a number of nuclides, are discretised using a finite volume discretisation in both the spatial and temporal dimensions. The resulting system of ordinary differential equations is then solved using the LSODE solver from the ODEPACK suite from the Lawrence Livermore National Laboratories (Hindmarsh 1983).

An overview of the different models and codes used by SKB is given in SKB (2010a).

1.2 About this user's guide

This manual is intended to be a guide for new users and a reference for more experienced users. The manual is intended to be as generic as possible. It is organised as follows:

- Chapter 1** gives an introduction to the program and how to read this guide.
- Chapter 2** details the theoretical background and the mathematical description.
- Chapter 3** presents a detailed description on how to run FARF33.
- Appendix A** describes the program structure, i.e. call sequence of subroutines/functions
- Appendix B** contains the test batch.

The guide is largely based upon Vahlund and Hermansson (2006).

2 Description of the model

The basis for the modelling is a stream tube, which in this case is a volume of rock including fractures with flowing water. The walls of the stream tube are defined by stream surfaces. As a consequence, no water is allowed to pass through walls of the stream tube and thus all mass entering one end of a stream tube will subsequently be discharged at the other end, assumed no radioactive decay occurs. FARF33 does not explicitly consider the transport in individual fractures and flow paths contained within the stream tube. Instead, the transport properties of the water-bearing fractures and the rock matrix available through diffusion are averaged over the stream tube, using the dual porosity continuum approach. The stream tube concept facilitates the radionuclide transport modelling. The complex three-dimensional flow field is thus divided into a set of one-dimensional stream tubes.

Figure 2-1 illustrates the transport of radionuclides through a fracture, and the interaction mechanisms.

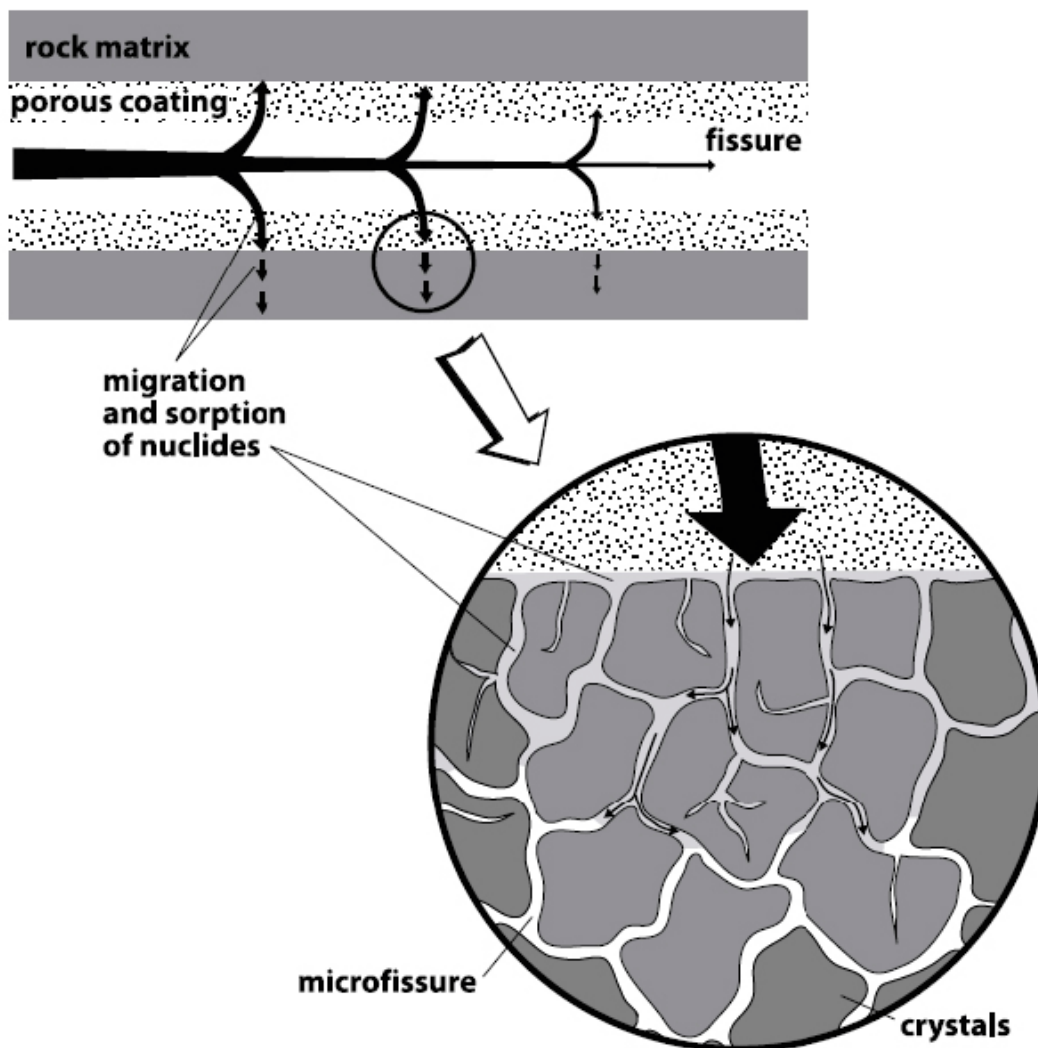


Figure 2-1. Matrix diffusion and sorption in the microfissures in the rock matrix (Redrawn from Lindgren et al. 2004).

2.1 Mathematical description

The physical quantities and the symbols used to denote them are listed in Table 2-1 for ease of reference.

Table 2-1. Quantities used in the mathematical description.

Parameter	Unit	Definition
u_s	[m a ⁻¹]	Darcy velocity
L	[m]	Stream tube length
t_w	[a]	Groundwater travel time
c_s^i	[mol m ⁻³]	Concentration of nuclide i in solute
c_p^i	[mol m ⁻³]	Concentration of nuclide i in pore water
D_s	[m ² a ⁻¹]	Solute dispersion coefficient; also represents molecular diffusion in the stream-wise direction
a_w	[m ⁻¹]	Total surface area per volume of mobile water at interface
D_e	[m ² a ⁻¹]	Effective matrix diffusivity
D_a	[m ² a ⁻¹]	Apparent matrix diffusivity
R^i	[-]	Retention factor of nuclide i
λ^i	[a ⁻¹]	Decay constant of nuclide i
ε	[-]	Matrix porosity
ρ_b	[kg m ⁻³]	Matrix bulk density
K_d^i	[m ³ kg ⁻¹]	Sorption coefficient of nuclide i
Pe	[-]	Peclet number
η	[-]	Solute injection fraction
c_m^i	[mol m ⁻³]	Concentration of nuclide i sorbed onto mobile colloids
c_f^i	[mol m ⁻³]	Concentration of nuclide i sorbed onto immobile colloids
κ_1	[a ⁻¹]	Rate of sorption/desorption on mobile colloids
κ_2	[a ⁻¹]	Rate of sorption/desorption on immobile colloids
k_1	[-]	Partition coefficient for nuclides sorbed to mobile colloids
k_2	[-]	Partition coefficient for nuclides sorbed to immobile colloids
β	[-]	Ratio of immobile to mobile colloids ($c_f^i = \beta c_m^i$, see Section 2.4)
u_m	[m a ⁻¹]	Advective flow rate of mobile colloids
D_m	[m ² a ⁻¹]	Dispersion coefficient for mobile colloids

The finite volume method is, like the finite difference method and the finite element method, a numerical scheme used to discretise the system of equations needed to solve, in the present implementation, a transport problem. Consider the conservation law for a scalar quantity c^i over an arbitrary volume Ω :

$$\frac{\partial}{\partial t} \int_{\Omega} c^i dV + \oint_S \mathbf{F} \cdot d\mathbf{S} = \int_{\Omega} Q dV, \quad (2-1)$$

using \mathbf{F} to represent fluxes over the boundaries S of the volume Ω and Q for volume sources. This integral representation simply reads that the change in the quantity c^i in the volume Ω corresponds to the flux over the boundaries S of Ω and the amount of the quantity that is generated or destroyed inside the volume. As noted above, no mass is allowed to pass through the walls of the stream tube, and consequently there is no surface source term. Applying Gauss' theorem on Equation 2-1 yields the differential form of the conservation law,

$$\frac{\partial c^i}{\partial t} + \nabla \cdot \mathbf{F} = Q, \quad (2-2)$$

which corresponds to that used in the FARF31 (Norman and Kjellbert 1990) and Collage II Plus codes.

By determining the fluxes (which in a diffusive/dispersive case are functions of the concentration gradient and in an advective case are functions of the concentration and advective velocity) and the sources as functions of the concentration, a system of equations on the form

$$\frac{\partial c^i}{\partial t} = f(c^i, t) \quad (2-3)$$

may be obtained. Initially, the problem is hence to express sources and fluxes on a form such that the conservation law may be written on a form corresponding to Equation 2-3. To do this, the conservation law for the sorbed nuclides, the nuclides migrating through the rock matrix and those migrating with the colloidal phase must be determined.

2.2 Implementing advection and dispersion in the stream tube

Nuclides dissolved in (and hence migrating with) the groundwater are modelled using the advection-dispersion equation. The flux vector \mathbf{F} in Equation 2-1 is hence written as the sum of an advective component $\mathbf{F}_A = c_s^i \mathbf{u}_s$ and a dispersive component $\mathbf{F}_D = -D_s \nabla c_s^i$, where \mathbf{u}_s represents the Darcy velocity, D_s the dispersion coefficient and c_s^i the concentration in the solute.

According to the stream tube conceptualisation, both the advective and dispersive fluxes are defined to be in the direction of the stream tube, which is defined to be the z -direction. Migration of the nuclides from the pore water into the rock matrix is also allowed, which is thought of as transport by diffusion in a transversal direction, defined to be the x -direction (perpendicular to the fracture in the Collage conceptualisation). Figure 2-2 illustrates the coordinate system, but note that this cylinder model is a simplification.

The fracture is very irregular. The transverse diffusive flux is hence handled by a volume source term introduced into Equation 2-1:

$$Q_s = a_w D_e \left. \frac{\partial c_p^i}{\partial x} \right|_{x=0}, \quad (2-4)$$

where a_w corresponds to the total surface area at the interface per volume of mobile water. Further, the effect of decay and in-growth may be written as a volume source term

$$Q_v = -\lambda c^i + \lambda^{i-1} c^{i-1}, \quad (2-5)$$

where λ represents the decay coefficient and the i and $i-1$ superscripts denote a nuclide and its mother nuclide. Note that this does not allow for branching decay chains. Including these terms in

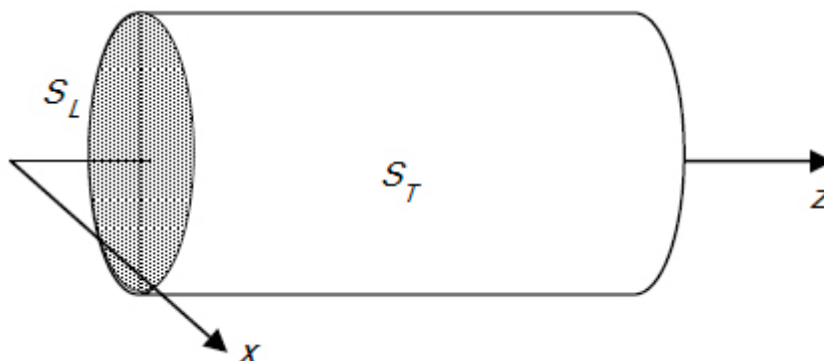


Figure 2-2. Coordinate system used to represent the stream tube conceptualisation. S_T is the surface boundary in the transverse direction, and S_L corresponds to the area in the longitudinal direction.

Equation 2-1, the integral form of the advection-dispersion equation with a transverse diffusion and nuclide decay may be written

$$\frac{\partial}{\partial t} \int_{\Omega} c_s^i dV + \oint_{S_L} \left(u_s c_s^i - D_s \frac{\partial c_s^i}{\partial z} \right) dS_L = \int_{\Omega} \left(a_w D_e \frac{\partial c_p^i}{\partial x} \Big|_{x=0} + \lambda^{i-1} c_s^{i-1} - \lambda^i c_s^i + Q_{\text{colloid}} \right) dV, \quad (2-6)$$

where Q_{colloid} represents the exchange term between the dissolved and colloidal phases (introduced in subsequent sections). S_L corresponds to the area in the longitudinal direction. Further, the boundary condition at the inlet boundary for Equation 2-6 may be expressed as

$$\frac{4\pi}{a_w^2} \left[u_s c_s^i \Big|_{\text{inlet}} - D_s \frac{\partial c_s^i}{\partial z} \Big|_{\text{inlet}} \right] = \eta \text{In}(t), \quad (2-7)$$

where $\text{In}(t)$ represents the time dependent inflow of nuclides (in units of mol a⁻¹) and η is the fraction of the inflow that occurs in the solute phase, as opposed to sorbed to colloids. $4\pi/a_w^2$ is the inlet factor for the fracture.

At the output boundary, $z = L$, two different boundary conditions have been implemented. The first is a homogenous boundary condition assuming zero concentration outside the downstream boundary. The second is a free boundary condition where the concentration outside the boundary is calculated using extrapolation and the out-flux is given by

$$\text{Out}(t) = \frac{4\pi}{a_w^2} \left[u_s c_s^i \Big|_{\text{outlet}} - D_s \frac{\partial c_s^i}{\partial z} \Big|_{\text{outlet}} \right]. \quad (2-8)$$

2.3 Implementing diffusion in the rock matrix

In addition to the longitudinal flux, modelled with the advection-dispersion equation, the nuclides are also assumed to be transported into the porous rock matrix adjacent to the fracture. Inside the matrix, nuclides will diffuse both in the water phase through the porous network and through surface diffusion in the solid rock. In the present implementation, only transverse flux (in the x -direction) is regarded and the diffusive flux F_p in the porous media is modelled using a 1D Fickian like model

$$F_p = -D_a^i \frac{\partial c_p^i}{\partial x}, \quad (2-9)$$

where c_p^i represents the concentration of nuclide i in the pore water and D_a corresponds to an apparent diffusivity coefficient which accounts for the lumped effect of porosity and sorption. Implementing a 2D diffusional model instead of a 1D is straightforward, but has not been done since it prevents accurate comparisons with the reference codes. Following the methodology used in the FARF31 code, the apparent diffusivity is related to the effective diffusivity

$$D_a = \frac{D_e}{R}, \quad (2-10)$$

where the retention factor R is expressed as

$$R^i = \varepsilon + K_d^i \rho_b, \quad (2-11)$$

being a function of the porosity ε , the sorption coefficient K_d^i (from which the concentration in the solid phase may be determined, $c_{\text{solid}} = K_d^i c_p^i$) and the bulk density of the rock ρ_b . Note that this definition differs from the retention coefficient in the Collage II Plus code and hence the definition of the apparent diffusivity. The differences between the definitions of the two codes are studied in more detail in Section 2.5. If the conservation equation is applied for a diffusive flux $F = F_p$, Equation 2-1 may be written

$$\frac{\partial}{\partial t} \int_{\Omega} c_p^i dV - \oint_{S} \frac{D_e^i}{R^i} \frac{\partial c_p^i}{\partial x} dS = \int_{\Omega} \left(\frac{R^{i-1}}{R^i} \lambda^{i-1} c_p^{i-1} - \lambda^i c_p^i \right) dV, \quad (2-12)$$

where the decay has been implemented as a volume source term in a corresponding way as in the advection-diffusion equation. In the present implementation, the following boundary conditions are used:

$$\begin{aligned} c_p^i &= c_s^i \quad \text{at the interface } x = 0, \\ \frac{\partial c_p^i}{\partial x} &= 0 \quad \text{at the interface } x = L_x, \end{aligned} \quad (2-13)$$

where L_x is the length to a symmetry boundary (half the length to the closest stream tube or fracture), also called the penetration depth.

An initial condition of $c_p^i = 0$ at $t = 0$ is used for the whole domain.

2.4 Implementing colloids

In addition to the solute transport, modelled using the advection-dispersion equation, colloid facilitated migration is also regarded as a possible migration mechanism for radionuclides. This is modelled in a way corresponding to that of Collage II Plus code where colloid facilitated migration was added as a source term in the advection-dispersion equation. In that implementation, nuclides were assumed to adsorb reversibly to colloids and to migrate with the colloids at an advection velocity not necessarily the same as that for the solute transport. In the Collage implementation, colloids were assumed to be either mobile or immobile (trapped in the fracture) and that there is a linear relation between the mobile and the immobile concentration.

In addition to a source term in the advection-dispersion equation, which represents transfer between the solute and the colloid phases, another transport equation is needed to model the mobile colloids. Consider the radionuclides sorbed onto mobile colloids:

$$\frac{\partial}{\partial t} \int_{\Omega} c_m^i dV + \oint_S \left(u_m c_m^i - D_m \frac{\partial c_m^i}{\partial z} \right) dS = \int_{\Omega} [\lambda^{i-1} c_m^{i-1} - \lambda^i c_m^i - \kappa_1 c_m^i + \kappa_1 k_1 c_s^i - q] dV, \quad (2-14)$$

where c_m corresponds to the concentration of nuclide i sorbed to mobile colloids, and an advective flow rate u_m and a dispersion coefficient D_m have been introduced for the colloid transport. The factors k_1 and k_2 are partition coefficients for radionuclides sorbed to mobile and immobile colloids, respectively. The factors κ_1 and κ_2 correspond to the rate of sorption-desorption onto mobile and immobile colloids, respectively. The quantity q represents the effective transport of radionuclides from mobile to immobile colloids resulting from colloids attaching to or releasing from the rock. For immobile colloids, we have

$$\frac{\partial}{\partial t} \int_{\Omega} c_f^i dV = \int_{\Omega} [\lambda^{i-1} c_f^{i-1} - \lambda^i c_f^i - \kappa_2 c_f^i + \kappa_2 k_2 c_s^i + q] dV, \quad (2-15)$$

where c_f represents the concentration of radionuclides sorbed onto immobile colloids. Like in the Collage model, it is assumed that the concentration of radionuclides per colloid is the same for both mobile and immobile colloids, which yields a linear relation that can be written $c_f^i = \beta c_m^i$, where β represents the ratio of immobile to mobile colloids (if $\beta = 0$, only mobile colloids exist). Equations 2-14 and 2-15 together can be combined to the following transport equation for radionuclides sorbed onto colloids:

$$\frac{\partial}{\partial t} \int_{\Omega} (1 + \beta) c_m^i dV + \oint_S \left(u_m c_m^i - D_m \frac{\partial c_m^i}{\partial z} \right) dS = \int_{\Omega} [\lambda^{i-1} (1 + \beta) c_m^{i-1} - \lambda^i (1 + \beta) c_m^i - (\kappa_1 + \beta \kappa_2) c_m^i + (\kappa_1 k_1 + \kappa_2 k_2) c_s^i] dV. \quad (2-16)$$

With the notation introduced previously, the additional source term Q_{colloid} added to the advection-dispersion equation becomes

$$Q_{\text{colloid}} = (\kappa_1 + \beta \kappa_2) c_m^i - (\kappa_1 k_1 + \kappa_2 k_2) c_s^i. \quad (2-17)$$

It should be noted that the partition parameters used in the Collage model, and consequently in the FARF33 model, are generally not what is reported in the literature. The derivation assumes that the partition coefficients for colloids can be written as

$$k_1 = K_p \alpha_m, \quad k_2 = K'_p \alpha_f, \quad (2-18)$$

where K_p and K'_p [$\text{m}^3 \text{kg}^{-1}$] are the distribution coefficients for radionuclides on mobile and immobile colloids (analogous to K_d), and α_m and α_f [kg m^{-3}] are the suspended load of mobile and immobile colloids, respectively (Klos et al. 2002).

The inlet boundary condition is implemented in a corresponding way as for the solute phase:

$$\frac{4\pi}{a_w^2} \left[u_m c_m^i \Big|_{\text{inlet}} - D_m \frac{\partial c_m^i}{\partial z} \Big|_{\text{inlet}} \right] = (1-\eta) \text{In}(t). \quad (2-19)$$

At the output boundary, at $z = L$, two different boundary conditions have been implemented. The first is a homogenous boundary condition assuming zero concentration outside the downstream boundary. The second is a free boundary condition, where the concentration outside the boundary is calculated using extrapolation and the out-flux is given by

$$\text{Out}(t) = \frac{4\pi}{a_w^2} \left[u_m c_m^i \Big|_{\text{outlet}} - D_m \frac{\partial c_m^i}{\partial z} \Big|_{\text{outlet}} \right]. \quad (2-20)$$

As for the solute phase, the initial condition that there are no nuclides present at $t = 0$ is used for the entire domain.

2.5 Comparison to variables used in the Collage code

The Collage code has been used as a reference code, but due to slight differences in the models and the notation, care must be taken when comparing the two.

The diffusivity used in Collage is the *pore* diffusivity, usually written D_p , while the FARF model uses *effective* diffusivity, usually written D_e . These two different diffusivities are related to each other according to

$$D_e = \varepsilon D_p. \quad (2-21)$$

The retention (or retardation) factor R is defined differently in the two models:

$$R_{\text{Collage}} = 1 + \frac{1-\varepsilon}{\varepsilon} K_d \rho_s, \quad (2-22)$$

$$R_{\text{FARF}} = \varepsilon + K_d \rho_b. \quad (2-23)$$

The density ρ_s in Collage is the *compact* density, while the FARF model uses the *dry bulk* density ρ_b . The two different densities are related to each other according to

$$\rho_b = (1-\varepsilon) \rho_s. \quad (2-24)$$

From equations 2-22–2-24 we obtain the relation

$$R_{\text{FARF}} = \varepsilon R_{\text{Collage}}. \quad (2-25)$$

2.6 A note on downstream boundary conditions

When using Laplace methods for the solutions, as in FARF31, it is possible to set a boundary condition for the concentration as the stream tube length or travel time goes to infinity. This possibility no longer exists in a finite volume discretisation where the computational domain must be finite. What boundary condition to use downstream in this case is really a modelling issue. Therefore, two different downstream boundary conditions are implemented. One approach is that the dilution is so large downstream of a certain model domain that the concentration can be neglected compared to the concentration inside the boundary. Using this assumption is equivalent to using the homogenous downstream boundary condition.

In the presence of colloids, it is likely that the solution curve will have two distinct peaks. Then it may be a better approximation to use an extrapolated boundary condition downstream to allow diffusion from the outside back into the computational domain, a situation that may occur between the two peaks. This corresponds to using the free boundary condition.

3 Simulation with FARF33

The input data to FARF33 is specified in the following files:

in.dat	General simulation data and definition of radionuclides and chains
in.par	Transport and physical parameter values
in.ts	The input time series
casename31.prm	Optional file specifying parameters for the numerical solution. 'casename' is specified by the user in the file 'in.dat'.

3.1 The input file 'in.dat'

The data specified is first some general data for the case assigned with keywords followed by the definition of the radionuclides and chains. The first section is read in free format. Comment lines and blank line are allowed. Comments begin with the character #. The keywords and values in Table 3-1 are recognised.

Table 3-1. Keywords for the input file 'in.dat'.

Keyword	Value	Description
PRINT	ON OFF DEBUG	Variable used to control what is written to standard output. The DEBUG value is accepted for compatibility reasons and functions exactly as ON.
CASENAME	casename	Name of the case and of the numerical parameter file 'casename31.prm'.
DIFFUSIVITY	SINGLE ELEMENT_SPECIFIC	Variable used to control if one single diffusion coefficient is used or if chemical element specific diffusion coefficients are used.

The second part of the file 'in.dat' includes the definition of the radionuclides and chains. The nuclides are specified on one line each, with the following data separated by whitespace:

- The name of the nuclide. The maximum length is 6 characters.
- The half-life of the nuclide, in years.
- A **1** if the nuclide has a daughter, and **0** otherwise.
- A **1** if there is an input time series for this nuclide, and **0** otherwise (in-growth only).

If a nuclide has a daughter, the definition of the daughter has to follow immediately after the mother nuclide.

3.2 The input file 'in.par'

The following is a list of the input parameters that FARF33 expects in the file 'in.par'. The data is assigned with keywords and is read in free format. Comment lines and blank lines are allowed. Comments begin with the character #. The keywords and values in Table 3-2 are recognised.

Table 3-2. Keywords of the input file ‘in.par’.

Keyword	Unit	Description
TW	[a]	Groundwater travel time over far field migration path (t_w). If TW < 0, empty single-point time series will be laid out.
PECLET	[-]	Longitudinal dispersion Peclet number (Pe).
ASPEC	[m ⁻¹]	Surface sorption area per unit of liquid volume in fractures (a_w).
F	[m ⁻¹ a]	F-factor ($t_w a_w$).
EPS	[-]	Matrix porosity, (ϵ).
DE	[m ² a ⁻¹]	Effective matrix diffusion coefficient, (D_e). Only given if DIFFUSIVITY is defined as SINGLE in the file in.dat.
PENDEP	[m]	Maximum depth of diffusive penetration into rock matrix.
ETA	[-]	Solute injection fraction for colloid transport (η).
BETA	[-]	Fraction of immobile colloids (β).
K1	[-]	Partition coefficient for radionuclides sorbing onto mobile colloids (k_1). See Equation 2-18.
K2	[-]	Partition coefficient for radionuclides sorbing onto immobile colloids (k_2). See Equation 2-18.
KAPPA1	[a ⁻¹]	Rate of sorption-desorption of mobile colloids (κ_1).
KAPPA2	[a ⁻¹]	Rate of sorption-desorption of immobile colloids (κ_2).
The following must be specified for each chemical element (not each nuclide). Note that an element is defined by the first two characters in the name of the nuclide. The elements must be specified in the same order as in the file ‘in.dat’. If there are several nuclides of the same element, it should only be specified once. The distribution coefficients must be given before the element-specific diffusion coefficients.		
KDR_XX	[m ³ kg ⁻¹]	Distribution coefficient (K_d) for element XX. Note that for chemical elements with only one letter also the first digit must be given, for example U2 for uranium.
DE_XX	[m ² a ⁻¹]	Effective matrix diffusion coefficient (D_e) for element XX. Only given if DIFFUSIVITY is defined as ELEMENT_SPECIFIC in the file ‘in.dat’. Note that for chemical elements with only one letter also the first digit must be given, for example U2 for uranium.

3.3 The input file ‘in.ts’

The input file ‘in.ts’ contains the input time series. The series must be given in the same order as in the definition of nuclides in the file ‘in.dat’. No time series should be included for those nuclides with in-growth only (specified in the file ‘in.dat’). Each time series starts with the name of the nuclide on the first line and thereafter the time series given with a time [a] and a migration rate from the near field in [mol a⁻¹] per line.

```
...
NUCLIDE
TIME MIGRATION-RATE
TIME MIGRATION-RATE
...
```

3.4 The numerical parameter file ‘casename31.prm’

Input from the optional file ‘casename31.prm’ sets parameters controlling the execution of the numerical algorithms, including the time steps and tolerance of the ODEPACK solver. The name of the file is due to historical reasons and is retained for compatibility with FARF31. Each line in the file must start with the name of the desired parameter followed by at least one space-character and then the value in free format.

```
...
PARAMETERNAME VALUE
...
```

Only those parameters that should be changed from their default values have to be specified in the file. Table 3-3 lists the recognised keywords.

Table 3-3. Keywords for the file ‘casename31.prm’.

Keyword	Default value	Description
MODE	log	Output series time point spacing mode. Valid values are log, lin or clg. clg in combination with NPMAX specifies a desired amount of output time series points. The line “MODE clg” should be placed at the top of the file.
NPMIN	32	Initial number of points in output time series.
NPMAX	128	Maximum number of points in output time series after truncation and densification.
DVARL	$1 \cdot 10^{-9}$	Left truncation limit of output series. First data point with value greater than $2 \cdot \text{DVARL} \cdot \text{MAX}$.
DVARR	$1 \cdot 10^{-6}$	Right truncation limit of output series. First data point with value greater than $2 \cdot \text{DVARR} \cdot \text{MAX}$.
RELINT	$1 \cdot 10^{-2}$	Maximum relative interpolation error in output time series.
BQMIN	$1 \cdot 10^{-3}$	Cutoff of Bq/a output. Anything smaller will be regarded as zero.
TSTART	0	Start time for the solution.
TSTOP	$5 \cdot 10^6$	Stop time for the solution.
TSTEP	1	Initial time step.
STPMIN	1	Minimum time step.
STPMAX	$1 \cdot 10^{10}$	Maximum time step.
RELTOL	$1 \cdot 10^{-3}$	Relative tolerance.
ABSTOL	$1 \cdot 10^{-6}$	Absolute tolerance.
NI	100	Number of cells in the stream-wise direction.
NJ	30	Number of cells in the transversal direction.
STRETCHING	4/3	Stretching factor for the mesh in the transversal direction.
LUDS	–	If present, use the upwind difference scheme (UDS) and the central difference scheme (CDS) otherwise.
LFREE	–	If present, use the free downstream boundary condition and the homogenous one otherwise.
ICOLL	1	The value 1 means that colloids should be present in the simulation and the value 0 means that there should be no colloids in the simulation.

The following keywords are considered obsolete for FARF33 and are recognised only for compatibility with FARF31: STEAMR, TALBOT, BROMEX, VARLS, VARRS, NPMINR, NPMAXR, MODER, DVARLR, DVARRR and RLNTR.

The output time series and the response time series are laid out by the PROPER times series manager (TSMGR). The time series manager first lays out NPMIN time points with logarithmic or linear spacing depending on the parameter MODE. The time series is first truncated in the beginning and at the end by removing values with relative magnitude less than $0.5 \cdot \text{DVARL}$ and $0.5 \cdot \text{DVARR}$, respectively. Additional points are then introduced in an iterative procedure in order to minimise the interpolation error. The target maximum interpolation error is given by RELINT. If the specified maximum interpolation error cannot be achieved with specified maximum number of points (NPMAX), the value of RELINT is doubled. The maximum absolute error in any point ERRACT is given in the extended output for debugging. If the value is 0, the target tolerance has not been exceeded. Values in the output time series less than BQMIN are removed. However, all output time series contain at least two points.

The truncation by the time series manager can be effectively minimised by specifying suitably small values for BQMIN, DVARL, DVARR and RELINT.

Example of a ‘casename31.prm’ file:

```
TSTART  0
TSTOP   1.0E9
NI       60
NJ       20
RELINT   1.0E-03
BQMIN    1.0E-10
```

3.5 Output

3.5.1 Time series output file 'out.ts'

The (truncated) output time series are sent to the file 'out.ts'. Each line has the format:

Time [a] Migration rate [mol a⁻¹] Migration rate [Bq a⁻¹]

3.5.2 Input echo file 'out.pr'

The main purpose of 'out.pr' is to record the assigned chemical element data, transport parameters and numerical parameters. The file contains information on the used input parameters from 'in.par'. Data such as half-lives, chain definition and source information comes from 'in.dat'. If the file '*casename31.prm*' is present, some of the numerical parameters are also written to this file.

3.5.3 Standard output

If the keyword PRINT is ON or DEBUG, information on the input parameters (from 'in.par') and numerical parameters are printed to standard output. Both numerical parameters assigned by the user in the file '*casename31.prm*' and the default values are given. Additionally, the full time series for the first nuclide in the chain is printed, which can be used to bypass the truncation.

References

SKB's (Svensk Kärnbränslehantering AB) publications can be found at www.skb.se/publications.

- Cvetkovic V, 2003.** Potential impact of colloids on plutonium migration at the Äspö site. SKB R-03-16, Svensk Kärnbränslehantering AB.
- Cvetkovic V, 2004.** Colloid-facilitated radionuclide transport in single fractures: Sensitivities and scoping calculations for tracer tests at Äspö. SKB R-04-49, Svensk Kärnbränslehantering AB.
- Hicks T W, 2003.** COLLAGE II Plus User's guide, Version 2. Galson Sciences Ltd.
- Hindmarsh A C, 1983.** ODEPACK: a systematized collection of ODE solvers. In Stepleman R S, Carver M (eds.) Scientific computing: applications of mathematics and computing to the physical sciences: proceedings of the 10th IMACS world congress on systems simulation and scientific computation, Montreal, Canada, 8–13 August 1982. Amsterdam: North-Holland, 55–64.
- Klos R A, White M J, Wickham S M, Bennett D G, Hicks T W, 2002.** Quantitative assessment of the potential significance of colloids to the KBS-3 disposal concept. SKI Report 02:34, Statens kärnkraftinspektion (Swedish Nuclear Power Inspectorate).
- Lindgren M, Gylling B, Elert M, 2002.** FARF31 Version 1.2 User's guide. SKB TS-02-03, Svensk Kärnbränslehantering AB.
- Lindgren M, Gylling B, Elert M, 2004.** Assessment model validity document FARF31. SKB R-04-51, Svensk Kärnbränslehantering AB.
- Norman S, Kjellbert N, 1990.** FARF31 – A far field radionuclide migration code for use with the PROPER package. SKB TR 90-01, Svensk Kärnbränslehantering AB.
- Painter S, Mancillas J, 2009.** MARFA version 3.2.2 user's manual: migration analysis of radionuclides in the far field. SKB R-09-56, Svensk Kärnbränslehantering AB.
- SKB, 2010a.** Model summary report for the safety assessment SR-Site. SKB TR-10-51, Svensk Kärnbränslehantering AB.
- SKB, 2010b.** Radionuclide transport report for the safety assessment SR-Site. SKB TR-10-50, Svensk Kärnbränslehantering AB.
- Vahlund F, Hermansson H, 2006.** A direct numerical approach to solving the transport equations for radionuclide transport in fractured rock. SKB R-04-50, Svensk Kärnbränslehantering AB.

Call sequence

The following table shows the subroutine structure of the program.

Routine	Description
MAIN33	Main routine
VERS31	Setup program version headers
HEAD31	Open and write headers on output files
EXIT31	Error processing
IDATE	Date
ITIME	Time
GETD31	Read information concerning the chains and elements from data file in.dat
UPCLEN	Input string processing
EXIT31	Error processing
GPRM31	Set values of numerically related parameters by default or read them from a data file
UPCLEN	Input string processing
EXIT31	Error processing
ECHO31	Output numerical parameters
GETP31	Place parameter data into COMMON
UPCLEN	Input string processing
EXIT31	Error processing
OUTPAR31	Echo parameters and close input echo file
CHHD31	Check first line of input time series file and write output header on standard output
UPCLEN	Input string processing
EXIT31	Error processing
TSIN31	Place input time series into COMMON
UPCLEN	Input string processing
EXIT31	Error processing
LSOD33	Solve the discretised problem
EXIT31	Error processing
DLSODE	ODEPACK solver LSODE
F33	Compute the ODE function
INFUNC	Inlet time series function
JAC33	Compute the jacobian
TSUT32	Final computation and output of the time series
TSMGR	Time series management service routine
TSTRU	Generation of a time series
TSDEN	Local densification of a time series
TSMGR2	Time series management service routine with user-defined number of points

Test batch

The test batch for FARF33 consists of six cases. The first two cases come from the test batch of FARF31 (Lindgren et al. 2002) and can be used to validate the agreement between the two codes. The next three are adapted from the Collage II Plus manual (Hicks 2003). The final case uses realistic data and input time series from SKB (2010b).

B.1 Case 1

This case is the same as problem 1 from the standard set of FARF31 test cases, that is a calculation for chain 4N+2 with an increased effective diffusivity for uranium. No colloids are present. The results agree well with the FARF31 results. It is noted that the early part of the FARF33 breakthrough curves are slightly on the pessimistic side.

B.1.1 in.dat

```
#
# Case 1 for FARF33
# File: in.dat                111118
#
PRINT ON
DIFFUSIVITY ELEMENT_SPECIFIC
CASENAME farf1-

# Nuclide   Thalf    Daughter  Source
Pu242      379000   1          1
U238       4.51E+09 1          1
U234       247000   1          1
Th230      80000    1          1
Ra226      1600     0          1
```

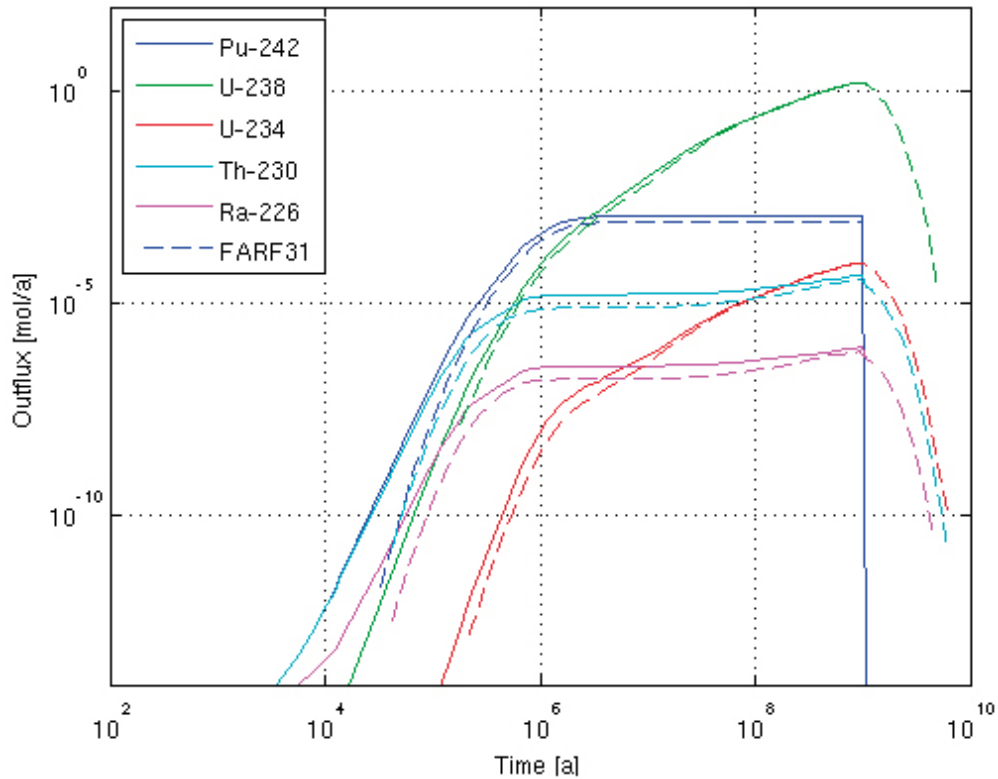


Figure B-1. Solution to case 1.

B.1.2 in.par

```
#
# Case 1 for FARF33
# File: in.par                111118
#
F          1.e5      # F = TW*ASPEC
TW         100.     # Groundwater travel time
PECLET     10.      # Peclet number
EPS        0.005    # Diffusion porosity of rock
PENDEP     2.0     # Depth of penetration
```

Chemical element information:

Kd values

KDR_Pu 1.

KDR_U2 1.

KDR_Th 1.

KDR_Ra 1.

Diffusion coefficients

DE_Pu 3.e-6

DE_U2 3.e-5

DE_Th 3.e-6

DE_Ra 3.e-6

B.1.3 in.ts

```
Pu242
1.0E2      1.0E-0
1.0E9      1.0E-0
U238
1.0E2      1.0E-0
1.0E9      1.0E-0
U234
1.0E2      1.0E-0
1.0E9      1.0E-0
Th230
1.0E2      1.0E-0
1.0E9      1.0E-0
Ra226
1.0E2      1.0E-0
1.0E9      1.0E-0
```

B.1.4 farf1-31.prm

```
#
# Case 1 for FARF33
# File: farf1-31.prm        111118
#
TSTART 0      # Start time for time integration
TSTOP 1.1e9   # Stop time for time integration
AbsTol 1e-6   # Absolute tolerance for time integration
RelTol 1e-3   # Relative tolerance for time integration
NI 60        # Number of points in streamwise direction
NJ 20        # Number of points in transversal direction
ICOLL 0      # No colloids

# Don't truncate so much
BQMIN 1e-20
DVARL 1e-20
DVARR 1e-20
RELINT 1e-20
```

B.2 Case 2

This case is the same as problem 2 of the FARF31 test batch. This example includes five hypothetical radionuclides that are designed to give the same output response. As for Case 1, it is noted that the early part of the FARF33 breakthrough curves are slightly on the pessimistic side.

B.2.1 in.dat

```
#
# Case 2 for FARF33
# File: in.dat                111118
#
PRINT ON
DIFFUSIVITY SINGLE
CASENAME farf2-
# Nuclide   Thalf   Daughter  Source
A1          1200000  1         1
B11         600000   1         1
B12         400000   1         1
C1          300000   1         1
D1          240000   0         1
```

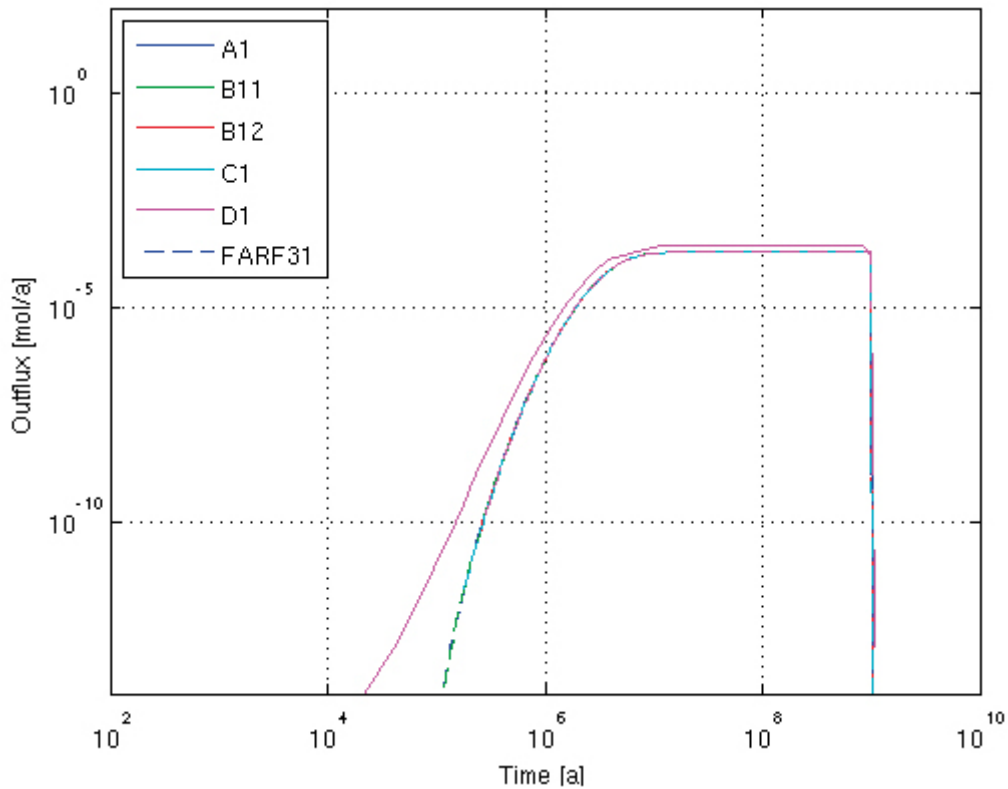


Figure B-2. Solution to case 2. The output series are identical for all nuclides.

B.2.2 in.par

```
#
# Case 2 for FARF33
# File: in.par                111118
#
F          1.e5      # F = TW*ASPEC
TW         100.     # Groundwater travel time
PECLET    10.      # Peclet number
EPS        0.005   # Diffusion porosity of rock
PENDEP    2.0      # Depth of penetration

# Chemical element information:
# Kd values
KDR_A1 5.
KDR_B1 5.
KDR_C1 5.
KDR_D1 5.
# Diffusion coefficients
DE 3.2E-6
```

B.2.3 in.ts

```
A1
1.0E2      1.0E-0
1.0E9      1.0E-0
B11
1.0E2      1.0E-0
1.0E9      1.0E-0
B12
1.0E2      1.0E-0
1.0E9      1.0E-0
C1
1.0E2      1.0E-0
1.0E9      1.0E-0
D1
1.0E2      1.0E-0
1.0E9      1.0E-0
```

B.2.4 farf2-31.prm

```
#
# Case 2 for FARF33
# File: farf2-31.prm        111118
#
TSTART 0      # Start time for time integration
TSTOP 1.1e9   # Stop time for time integration
AbsTol 1e-6   # Absolute tolerance for time integration
RelTol 1e-3   # Relative tolerance for time integration
NI 60        # Number of points in streamwise direction
NJ 20        # Number of points in transversal direction
ICOLL 0      # No colloids
# Don't truncate so much
BQMIN 1e-20
DVARL 1e-20
DVARR 1e-20
RELINT 1e-20
```

B.3 Case 3

This case is based upon the Collage problem C000 and is a test case with no radioactive decay and no colloids. The input time series consists of a single Dirac pulse at $t = 0$, which is approximated with a short pulse of finite length. As it has no colloids, it can also be verified against FARF31.

B.3.1 in.dat

```
#
# Case 3 for FARF33
# File: in.dat           111118
#
PRINT DEBUG
DIFFUSIVITY SINGLE
CASENAME C000-
# Nuclide   Thalf   Daughter  Source
A1         1.0e15   0         1
```

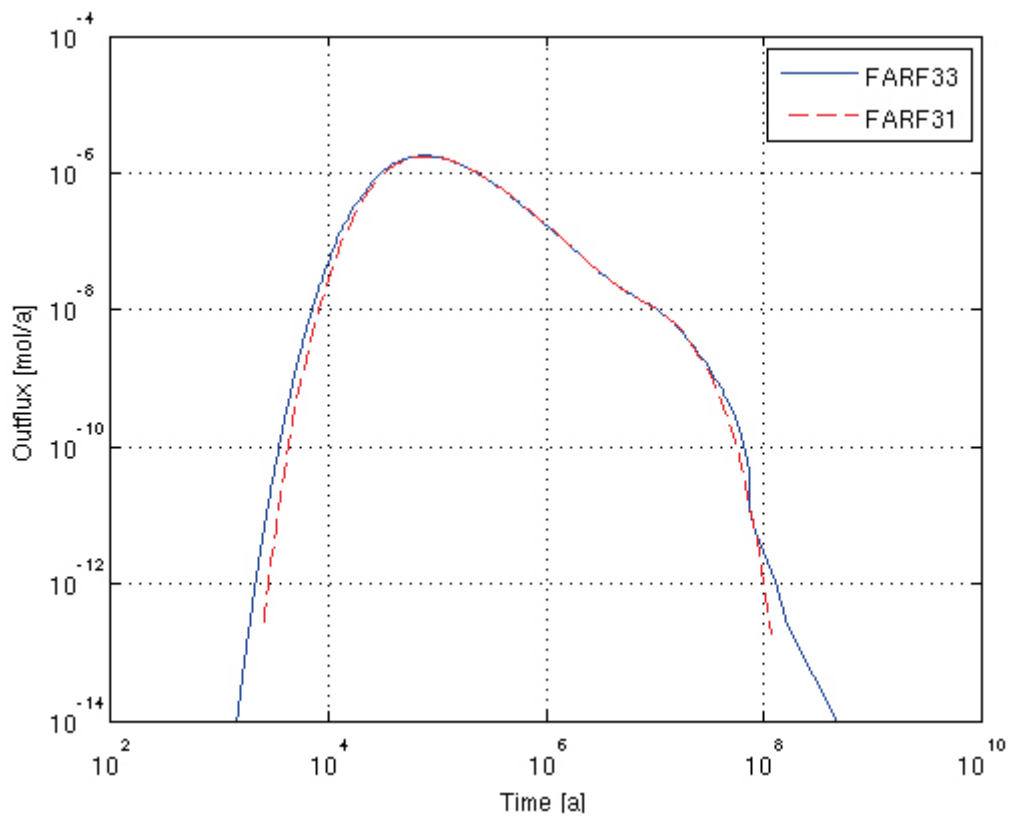


Figure B-3. Solution to case 3.

B.3.2 in.par

```
#
# Case 3 for FARF33
# File: in.par                111118
#
TW      1000    # Groundwater travel time
PECLET  50      # Peclet number
ASPEC   1       # Specific surface
EPS     0.01   # Diffusion porosity of rock
PENDEP  5.0    # Depth of penetration
```

Chemical element information:

```
KDR_A1 0.25    # Kd value
DE 7.875e-4    # Diffusion coefficient
```

Colloid parameters

```
BETA 0
ETA 1
K1 0
K2 0
KAPPA1 0
KAPPA2 0
```

B.3.3 in.ts

```
A1
0.0E0    1.0E6
1.0E-6   1.0E6
```

B.3.4 C000-31.prm

```
#
# Case 3 for FARF33
# File: C000-31.prm          111118
#
TSTART 0      # Start time for time integration
TSTOP 1e9     # Stop time for time integration
AbsTol 1e-6   # Absolute tolerance for time integration
RelTol 1e-3   # Relative tolerance for time integration
NI 100       # Number of points in streamwise direction
NJ 30        # Number of points in transversal direction
ICOLL 0      # No colloids
```

Don't truncate so much

```
BQMIN 1e-20
DVARL 1e-20
DVARR 1e-20
RELINT 1e-20
```

B.4 Case 4

This case is based upon Collage problem C997, and is a case with a slow sorption-desorption rate between mobile and immobile colloids. The case calculated with FARF33 is in good agreement with the calculations with Collage II Plus.

B.4.1 in.dat

```
#
# Case 4 for FARF33
# File: in.dat                111118
#
PRINT ON
DIFFUSIVITY SINGLE
CASENAME C997-
# Nuclide   Thalf   Daughter   Source
A1          1.0e15   0          1
```

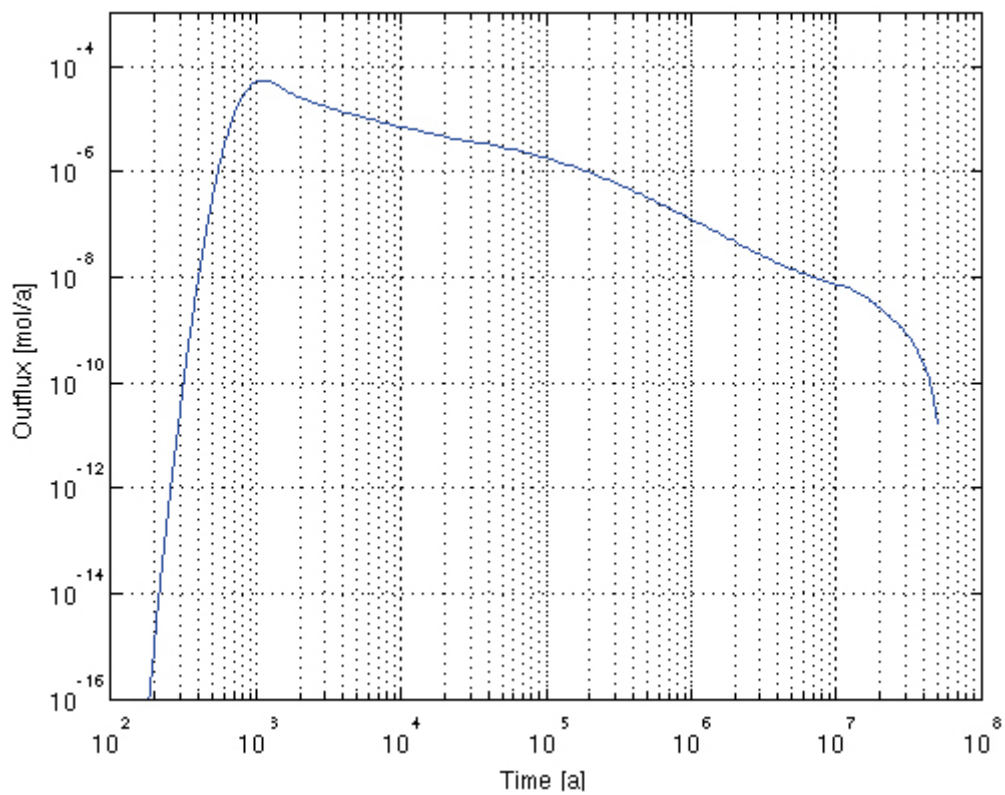


Figure B-4. Solution to case 4.

B.4.2 in.par

```
#
# Case 4 for FARF33
# File: in.par                111118
#
TW      1000    # Groundwater travel time
PECLET  50      # Peclet number
ASPEC   1       # Specific surface
EPS     0.01   # Diffusion porosity of rock
PENDEP  5.0    # Depth of penetration

# Chemical element information:
KDR_A1 0.25    # Kd value
DE 7.875e-4   # Diffusion coefficient

# Colloid parameters
BETA 0
ETA 1
K1 1.0e3
K2 0
KAPPA1 1e-6
KAPPA2 1e-6
```

B.4.3 in.ts

```
A1
0.0E0    1.0E6
1.0E-6   1.0E6
```

B.4.4 C997-31.prm

```
#
# Case 4 for FARF33
# File: C997-31.prm        111118
#
TSTART 0    # Start time for time integration
TSTOP 1e9   # Stop time for time integration
AbsTol 1e-6 # Absolute tolerance for time integration
RelTol 1e-3 # Relative tolerance for time integration
NI 100     # Number of points in streamwise direction
NJ 30      # Number of points in transversal direction
ICOLL 1    # Colloids are present

# Don't truncate so much
BQMIN 1e-20
DVARL 1e-20
DVARR 1e-20
RELINT 1e-20
```

B.5 Case 5

This case is based upon the Collage problem C999. The case has colloids and a fast sorption-desorption rate. The case calculated with FARF33 is in good agreement with the calculations with Collage II Plus.

B.5.1 in.dat

```
#
# Case 5 for FARF33
# File: in.dat                111118
#
PRINT ON
DIFFUSIVITY SINGLE
CASENAME C999-
# Nuclide    Thalf    Daughter    Source
A1          1.0e15    0           1
```

B.5.2 in.par

```
#
# Case 5 for FARF33
# File: in.par                111118
#
TW          1000.    # Groundwater travel time
PECLET      50      # Peclet number
ASPEC       1.      # Specific surface
EPS         0.01    # Diffusion porosity of rock
PENDEP     5.0     # Depth of penetration

# Chemical element information:
KDR_A1 0.25      # Kd value
DE 7.875e-4     # Diffusion coefficient

# Colloid parameters
BETA 0
ETA 1
K1 1.0e3
K2 0
KAPPA1 1.0
KAPPA2 1e-6
```

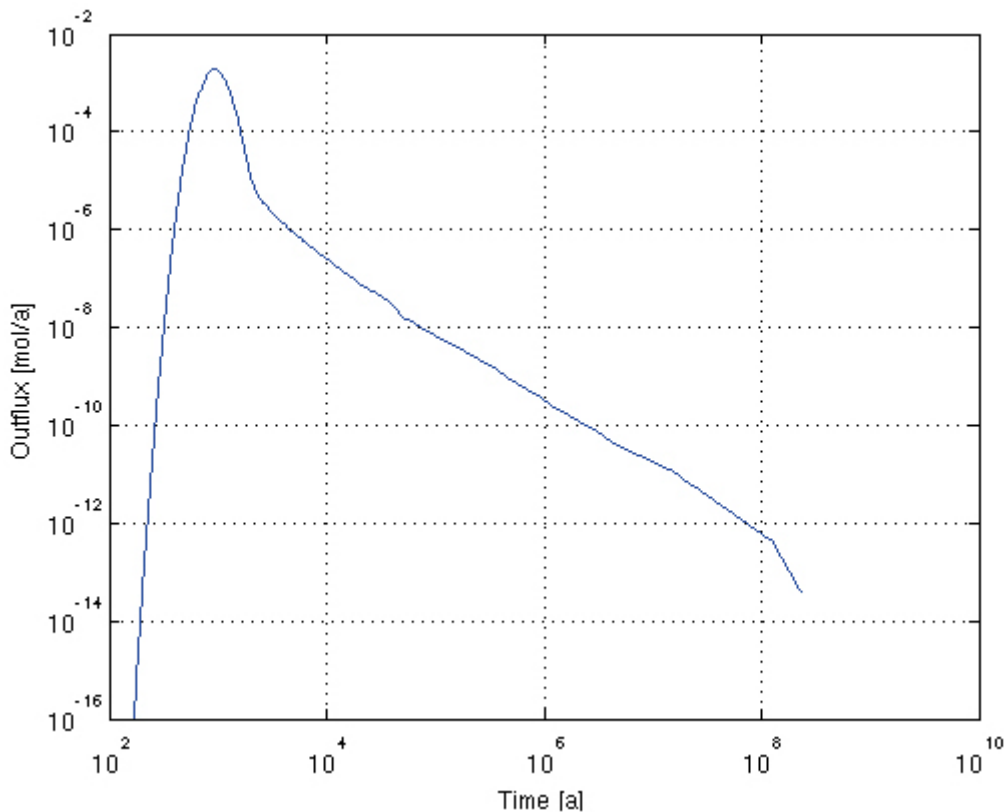


Figure B-5. Solution to case 5.

B.5.3 in.ts

```
A1
0.0E0      1.0E6
1.0E-6     1.0E6
```

B.5.4 C999-31.prm

```
#
# Case 5 for FARF33
# File: C999-31.prm          111118
#
TSTART 0 # Start time for time integration
TSTOP 1e9 # Stop time for time integration
AbsTol 1e-6 # Absolute tolerance for time integration
RelTol 1e-3 # Relative tolerance for time integration
NI 100 # Number of points in streamwise direction
NJ 30 # Number of points in transversal direction
ICOLL 1 # Colloids are present

# Don't truncate so much
BQMIN 1e-20
DVARL 1e-20
DVARR 1e-20
RELINT 1e-20
```

B.6 Case 6

This case is based upon realistic parameters and input time series for Pu-242 from the near-field calculations for central corrosion case in SR-Site (SKB 2010b). Two different levels of colloid concentration are simulated, 10 mg/L and 10 g/L, as well with no colloids at all. Calculations with the far field code MARFA (Painter and Mancillas 2009) are also plotted in the same figure for comparison.

B.6.1 in.dat

```
#
# Case 6 for FARF33
# File: in.dat          111118
#
PRINT ON
DIFFUSIVITY SINGLE
CASENAME SRSite
# Nuclide   Thalf      Daughter  Source
Pu242      3.733E+05  0         1
B.11.3     in.par
#
# Case 6 for FARF33
# File: in.par          111118
#
TW         6          # Groundwater travel time
PECLET     10         # Peclet number
F          53660      # F-factor
EPS        0.0018   # Diffusion porosity of rock
PENDEP     12.5     # Depth of penetration

# Chemical element information:
KDR_PU 1.5e-2 # Kd value
DE      6.3e-7 # Diffusion coefficient
```

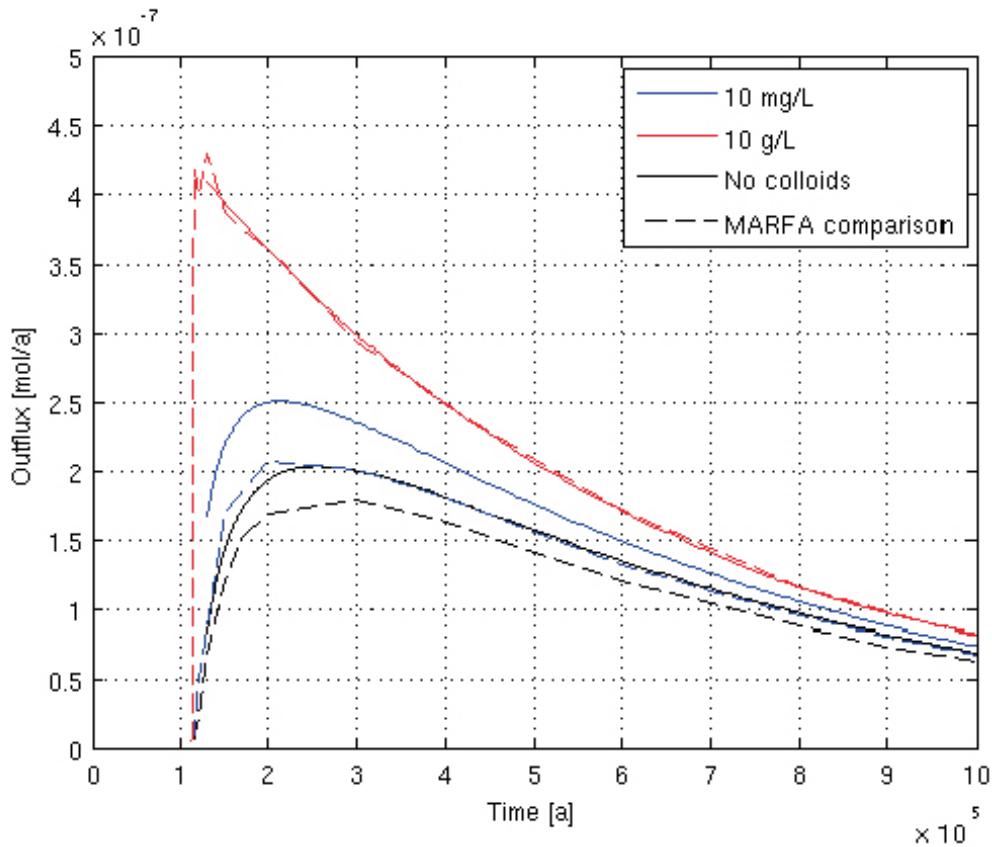


Figure B-6. Solution to case 6. The output from the simulation with high colloid concentration very closely resembles the input time series.

Colloid parameters

BETA	0	# No immobile colloids
ETA	0	# No immobile colloids
K1	0.39	# For high concentration case: 390
K2	0	# No immobile colloids
KAPPA1	1	# Rapid sorption-desorption rate of mobile colloids
KAPPA2	0	# No immobile colloids

B.6.3 in.ts

The complete input time series is too large to be given here, but is plotted in Figure B-7.

B.6.4 SRSite31.prm

```

#
# Case 6 for FARF33
# File: SRSite31.prm
#
TSTART 0
TSTOP 1e9
ABSTOL 1e-8
RELTOL 1e-5
NI 200
NJ 30
ICOLL 1
BQMIN 1e-20
DVARL 1e-20
DVARR 1e-20
RELINT 1e-30
NPMAX 2048
111118

```

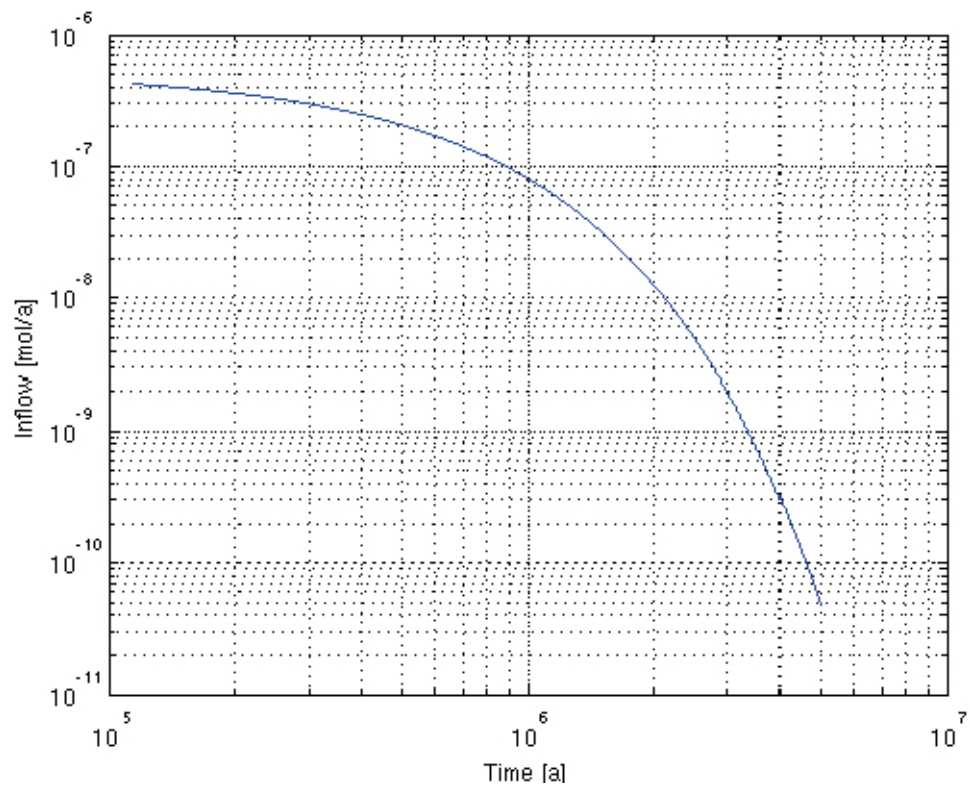


Figure B-7. The input time series for case 6.