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ARDISC (Argonne Dispersion Code): Computer Programs to Calculate the Distribution of Trace Element Migration in Partially Equilibrating Media

by

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Chemistry Division

April 1979

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Abstract

A computer program (ARDISC, the Argonne Dispersion
Code) is described which simulates the migration of
nuclides in porous media and includes first order
kinetic effects on the retention constants. The code
allows for different absorption and desorption rates
and solves the coupled migration equations by arithmetic
reiterations. Input data needed are the absorption
and desorption rates, equilibrium surface absorption
coefficients, flow rates and volumes, and media
porosities.

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The ability to predict the migratory behavior of trace

elements in the geosphere is a necessary prerequisite to the

construction of safe geological repositories for radioactive

waste materials. It has generally been assumed that this

migratory behavior will be described by equilibrium

chromatographic equations.

However, laboratory studies involving tracer amounts of

radioisotopes (Ref. 1,2,3) have shown that the sorption

processes are not necessarily reversible or at equilibrium

under geological conditions and that these conditions affect

the migratory behavior of various radionuclides.

This code was written to provide a method of investigating

these non-equilibrium effects by reducing their description

to a few basic parameters, which can be determined by

empirical means.

The common models for the migration and sorption of

solute between solid and solution phases are usually in the

form of differential equations (4-9). For example, in a

one-dimensional model using a uniformly porous medium, the convective dispersion of a solute (such as a radioactive tracer in solution) is given by

$$\frac{\partial S(x,t)}{\partial t} = \frac{D\partial^2 S(x,t)}{\partial x^2} - \frac{v\partial S(x,t)}{\partial x} - \frac{\beta}{\theta}\frac{\partial R(x,t)}{\partial t}$$

$$- \lambda[S(x,t) + R(x,t)] \qquad (1)$$

where:

S(x,t) = concentration of the solution at position x and time t. (mass per unit volume of solution phase)

R(x,t) = concentration of the sorbed species at position x and time t. (mass per unit mass of solid phase)

D = hydrodynamic dispersion coefficient

v = water velocity, assumed to be constant

β = bulk density

θ = porosity of medium

λ = 1st order radioactive decay constant of species, if it is a radioisotope.

If equilibrium is assumed, then R is a function of S. A common equilibrium model is the linear Freundlich isotherm,

$$R(x,t) = \frac{\theta}{\beta} k_3 S(x,t) \qquad (2)$$

where k_3 = dimensionless equilibrium constant. This

equation is valid where $R(x,t)$ does not approach saturation limits. If complete equilibrium is not assumed and irreversible conditions exist, then the relationship between R and S becomes more complicated and the solution for the differential equation (1) becomes a complex integral. For further details on the mathematical solutions of such equations, see references 6 and 10.

In the model discussed in this paper, a recursive approach is taken to determine the amount of a radiotracer sorbed on a rock column or the amount remaining in solution as a function of the time and distance from the source. This is a one-dimensional approach and assumes a constant velocity of solution through a uniform rock medium. Furthermore, no hydraulic dispersion is considered and the radioactive decay constant is set to zero.

BASIC DESCRIPTION OF MODEL

A one-dimensional column is divided into an arbitrary number (LEND) of units or zones. Each zone can sorb a solute such that at equilibrium the distribution of the species between the surface of the zone and the volume of solution (initially at unit concentration of species) is α/β, where α = the amount of species on the surface, and $\beta = 1 - \alpha$.

If, after this distribution exists, a second cycle

occurs in which the solution from the initial zone is transferred to a second zone with the same sorption characteristics and a fresh solution containing none of the solute is placed in the first zone, another equilibration, this time in both zones, will occur. This process would be repeated for additional cycles and zones. Thus after a given number of cycles (C), for a particular zone (Z), the following relationship would exist:

$$R(C,Z) = \alpha[R(C-1,Z) + S(C-1,Z)] \qquad (3)$$

$$S(C,Z+1) = \beta[R(C-1,Z) + S(C-1,Z)] \qquad (4)$$

where:

> $R(C,Z)$ = fractional amount of material (relative to some scaling value) sorbed on the Zth zone after the Cth cycle.

> $S(C,Z+1)$ = fractional amount of material (relative to the scaling value used above) in solution in the (Z+1) zone after the Cth cycle.

$S(C,Z+1)$ is the solution which was equilibrated in zone Z during cycle C and transferred to zone (Z+1) at the end of cycle C. Depending on the value of $S(C,0)$ for $C \geq 0$, the input of solute to the column may be in the form of a pulse or a continuous feeding. $R(C,0) = 0$ is assumed for all C.

If the movement from zone to zone were fast enough such that complete equilibrium in each zone did not occur, one could designate an arbitrary fraction of the tracer initially in solution reaching equilibrium, F, where:

$$F(t) = \frac{\text{fraction of tracer sorbed from solution during a cycle time, } t}{\text{fraction of tracer sorbed from solution at equilibrium} } \quad (5)$$

For the tracer which is initially on the surface of the zone, one could designate an arbitrary fraction of the tracer reaching a desorbing equilibrium, G, where

$$G(t) = \frac{\text{fraction of tracer desorbed from the surface during a cycle time, } t}{\text{fraction of tracer desorbed from the surface at equilibrium}} \quad (6)$$

The determination of F and G values for a particular cycle time must be determined in kinetic sorption and desorption experiments.

For each particular zone, during a given cycle, the sorption-desorption process is separated into two distinct paths with either F or G involved in each path. Such an approach incorporates a first order rate toward equilibrium. While it is probably not likely that the complicated chemistry of sorption is a first order process, such an approximation is valid if one is dealing with tracer concentrations of the solute and the concentration of sorption sites remains constant (i.e., saturation is not achieved).

If a cycle is now defined as a partial equilibration

between the tracer and the zone surface, followed by an instantaneous transfer of the solution to the next zone, the following recursive formulae apply (see Figure 1):

$$R(C,Z) = G\alpha R(C-1,Z) + (1-G)R(C-1,Z) + F\alpha S(C-1,Z) \qquad (7)$$

$$S(C,Z+1) = F\beta S(C-1,Z) + (1-F)S(C-1,Z) + G\beta R(C-1,Z) \qquad (8)$$

or, rearranging

$$R(C,Z) = [G\alpha+1-G]R(C-1,Z) + F\alpha S(C-1,Z) \qquad (9)$$

$$S(C,Z+1) = [F\beta+1-F]S(C-1,Z) + G\beta R(C-1,Z) \qquad (10)$$

where, $R(C,Z)$ = fractional amount of tracer sorbed on the surface in the Zth zone after the Cth cycle

$S(C,Z+1)$ = fractional amount of tracer in solution in the (Z+1)th zone during the Cth cycle.

For a mathematical discussion of $R(C,Z)$ and $S(C,Z+1)$, see Appendix A.
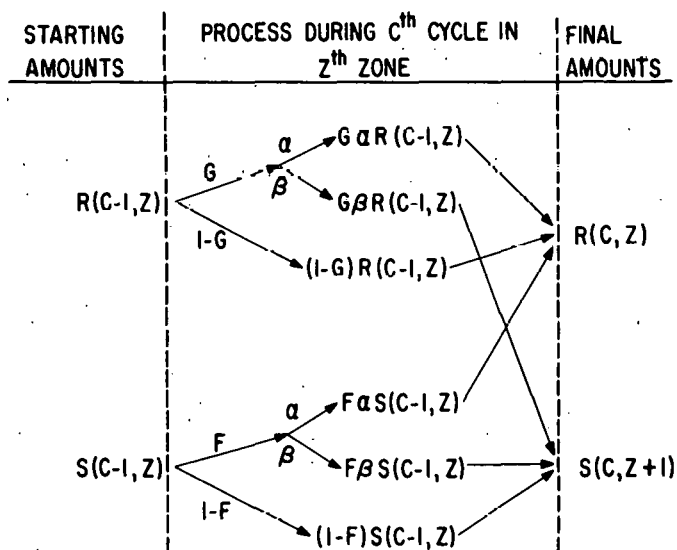

Figure 1

ARDISC (Argonne Distribution Code) and ARDISC 1 are two FØRTRAN programs to calculate the distribution of a radioisotope in zones of partially equilibrated rock. The number of zones, the number of cycles and the amount of applied tracer can be specified in the program input along with various sorption, equilibration, and other factors. The output consists of a listing of the distribution of the tracer on the rock zones, and in the zone solutions, as well as cumulative totals of each. Other options such as a plot of the distribution and zone grouping may also be employed and are discussed below. Both input and output involve dimensionless numbers, so that a conversion to concentration (either molar or molal) would require an additional subroutine to alter the final arrays of R and S values.

The difference between ARDISC and ARDISC 1 is in the number of zones which are involved in the distribution analysis. Using ARDISC, only the rock zones are computed and listed in the print-out. Any tracer passing out of the final rock zone is dropped from the calculation. Using ARDISC 1, both rock zones and transfer zones (where no sorption occurs) are computed. The number of transfer zones is equal to the total number of cycles (MAXL) minus the total number of rock zones (LEND).

The Program Control Cards (Data Cards) consist of an initial rock specification card of the form:

Columns	Type	Variable	Description
1-10	F10.0	RA	The radius of a spherical zone, in cm. Default = 1.
11-20	F10.0	POR	The porosity of the rock, as a fraction. Default = 1.
21-30	F10.0	DEN	The density of the rock, in g/cm^3. Default = 1.
31-40	F10.0	ATIME	The total time for all cycles, in sec. Default = 1.
80	I1	NOERR	=0 or blank; suppresses certain IBM error messages. $\neq 0$; no suppression of IBM error messages.

None of the above variables are necessary for a migration calculation; but they are necessary for additional informative calculation at the end of each print-out which may be useful. The values given in the 1st card apply to all calculations in the job.

The second program control card is the one which contains the information needed for a migration calculation. For additional migration calculations using different migration characteristics or options, separate cards of the same format must be inserted directly behind the second program control card. The format of the second program control card is as follows:

Columns	Type	Variable	Description
1-10	F10.0	AMAXL	The number of cycles in the calculation. In ARDISC 1, this also specifies the total number of zones computed. In the programs, MAXL = AMAXL.
11-15	F5.0	ALEND	The number of zones in which the rock-solution sorption-desorption mechanism takes place. In ARDISC 1, the remaining AMAXL-ALEND zones are treated as transfer zones only. In both programs, LEND = ALEND and LEND must be less than or equal to MAXL.
16-20	F5.0	AKM	The number of zones in a group. In print-out and plotting, the tracer distributions and sums are listed for groups of zones, to save space. For ARDISC, ALEND/AKM must be an integer value; for ARDISC 1, AMAXL must be an integer.
21-25	F5.5	F	The fraction of the tracer initially in a zone solution reaching an equilibrium distribution during a cycle time.

Columns	Type	Variable	Description (cont'd)
26-30	F5.5	G	The fraction of the tracer initially on the zone surface reaching an equilibrium distribution during a cycle time.
31-35	F5.5	AL	The fraction of a tracer sorbed on the zone surface at equilibrium.
36-40	F5.0	S0	The number of units of tracer fed into the solution on the first zone for each cycle. This corresponds to a continuous, constant leaching of tracer from a source.
41-45	F5.0	S1	The number of units of tracer initially present in the first zone at the start of the first cycle. During subsequent cycles, no activity is fed into the 1st zone from an outside source.
46-50	F5.0	SWTCH	The cycle number at which the value of S0 is changed. Default: Option is not used.
51-55	F5.0	SSWT	The value of S0 beginning at cycle 'SWTCH'.

Columns	Type	Variable	Description (cont'd)
56-60	F5.0	PLØT	The type of plotting option desired. = 0 : No plot = 1 : R values are plotted as a fxn of group number = 2 : S values are plotted as a fxn of group number
61-65	F5.0	SAT	Limit on the number of units of tracer which can be sorbed on a zone surface; if SAT = 0 or blank, saturation limits are ignored.
66-70	F5.0	STRT	The initial value of R(C,Z) and S(C,Z) for all zones. Default = 0.

The usefulness of SAT is limited by the fact that as saturation becomes important, the kinetics of the sorption and desorption reactions are not likely to be 1st order, and the F and G value would be dependent on concentration. However, in ARDISC, the F and G values are fixed.

Currently (29 Aug 78) the two ARDISC programs are located on catalog disk data set at the Applied Mathematics Division, Argonne National Laboratory. The ARDISC program is limited to a maximum ALEND value of 20,000. The ARDISC 1 program is limited to a maximum AMAXL value of 20,000. The time required to run a migration calculation for MAXL = 5000

and LEND = 100 on ARDISC is approximately 2 seconds. The
time required by ARDISC 1 is approximately proportional to
$MAXL^2/2$). The time for ARDISC is approximately proportional
to $LEND \cdot MAXL - LEND^2/2$. A rough approximation to a time
estimate for the computation is

$$T = f \cdot \frac{MAXL^2}{2} \quad \text{for ARDISC 1}$$

or

$$T = f \left[LEND \cdot MAXL - \frac{LEND^2}{2} \right] \quad \text{for ARDISC}$$

where $f \sim 4 \times 10^{-6}$ sec.

The job cards needed to run the ARDISC or ARDISC 1
program are as follows:

Card No.

1. //Jobname   JØB   (Facctno,ℓℓ,,tt),REGIØN=400K, -
    PRTY=p,CLASS=C

2. Accounting Card (see AMD Users Guide for details)

3. //Stepname EXEC PGM=program {see below}

4. //STEPLIB DD DISP=SHR,DSN=C120.B26114.ZONKER

5. //FT06F001 DD SYSØUT=A

6. //FT05F001 DD *

Data Control Deck
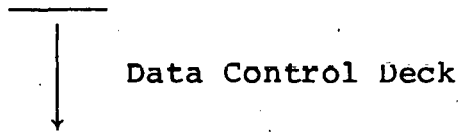
7. /* END OF FILE

$\ell\ell$ = thousands of lines of output estimated

tt = number of minutes of CPU time estimated

p = priority (see AMD User's Guide)

Program $\begin{cases} \text{For ARDISC, PGM = DRIPPER} \\ \text{For ARDISC 1, PGM = DRIPPER 1} \end{cases}$

An ARDISC program exists which can handle a value of AMAXL $\leq$ 50000; it can be called by using PGM = DRIPPER5. However, it requires that REGION = 700K.

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2. Sherman Fried, Arnold Friedman, Donald Cohen, John J. Hines, and Richard Strickert, "The Migration of Long-Lived Radioactive Processing Wastes in Selected Rocks," Annual Report to the Office of Waste Handling Project AN0115A, FY1977, ANL-78-46, Argonne National Laboratory, (1978).

3. Richard Strickert, Sherman Fried, Arnold Friedman, "The Sorption of Technetium and Iodine Radioisotopes by Various Minerals," Nuclear Technology, submitted for publication (1978).

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5. L. Lapidus and N. R. Amundson, J. Phys. Chem. 56, 984-958 (1952).

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8. F. T. Lindstrom, Water Resources Research 12(2), 229-238 (1976).

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APPENDIX A

The mathematical description of solute flow through a one-dimensional column divided into an arbitrary number of zones is discussed by Glueckauf (1), and is followed (with some modifications) for the ARDISC model. To simplify matters, dimensionless numbers are used:

C = cycle number

Z = zone number

$R(C,Z)$ = fractional amount of material (relative to some scaling value) sorbed on the Zth zone after the Cth cycle

$S(C,Z+1)$ = fractional amount of material in solution in the (Z+1) zone after the Cth cycle. (The solution was transferred from the Zth zone at the end of the Cth cycle, by convention.)

For material balance to occur, an <u>increase</u> in the material sorbed on the surface of the Zth zone after a cycle change, must be equal to a <u>decrease</u> in the material in the zone solution after the same cycle change.

$$\Delta R / \Delta C = -\Delta S / \Delta C \qquad \text{(A-1)}$$

For an arbitrarily small cycle change,

$$R(C,Z) - R(C-1,Z) = S(C-1,Z) - S(C,Z+1) \qquad \text{(A-2)}$$

Again, the term $S(C,Z+1)$ is used since, by convention, the solution is transferred to the next zone at the end of each cycle.

Using a Taylor Series Expansion,

$$R(C-1,Z) = R(C,Z) - \left(\frac{\partial R}{\partial C}\right)_Z + \frac{1}{2}\left(\frac{\partial^2 R}{\partial C^2}\right)_Z - \ldots \qquad \text{(A-3a)}$$

$$S(C-1,Z) = S(C,Z) - \left(\frac{\partial S}{\partial C}\right)_Z + \frac{1}{2}\left(\frac{\partial^2 S}{\partial C^2}\right)_Z - \ldots \qquad \text{(A-3b)}$$

$$S(C,Z+1) = S(C,Z) + \left(\frac{\partial S}{\partial Z}\right)_C + \frac{1}{2}\left(\frac{\partial^2 S}{\partial Z^2}\right)_C + \ldots \qquad \text{(A-3c)}$$

where $R = R(C,Z)$ and $X = S(C,Z)$.

Higher order differentials are negligible provided that the cycle and zone changes are small relative to the final maximum C and Z values.
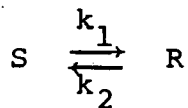
Substituting (A-3) into (A-2) gives

$$\left(\frac{\partial R}{\partial C}\right)_Z - \frac{1}{2}\left(\frac{\partial^2 R}{\partial C^2}\right)_Z - -\left(\frac{\partial S}{\partial C}\right)_Z + \frac{1}{2}\left(\frac{\partial^2 S}{\partial C^2}\right)_Z - \left(\frac{\partial S}{\partial Z}\right)_C - \frac{1}{2}\left(\frac{\partial^2 S}{\partial Z^2}\right)_C \qquad \text{(A-4)}$$

or rearranged to give

$$\left(\frac{\partial S}{\partial C}\right)_Z + \left(\frac{\partial R}{\partial C}\right)_Z - \frac{1}{2}\left(\frac{\partial^2 S}{\partial Z^2}\right)_C - \frac{1}{2}\left[\left(\frac{\partial^2 S}{\partial C^2}\right)_Z + \left(\frac{\partial^2 R}{\partial C^2}\right)_Z\right] + \left(\frac{\partial S}{\partial Z}\right)_C = 0 \qquad \text{(A-5)}$$

For a first order reversible rate reaction

$$S \; \underset{k_2}{\overset{k_1}{\rightleftharpoons}} \; R$$

where k_1 and k_2 are the sorption and desorption rate constants, one can write

$$\frac{dR}{dC} = k_1'S - k_2'C \qquad \text{(A-6)}$$

where k_1 and k_2 are the dimensionless rate constants

$$k_1' = \frac{k_1}{k_1 + k_2} \qquad \text{(A-7)}$$

$$k_2' = \frac{k_2}{k_1 + k_2} \qquad \text{(A-8)}$$

For the Zth zone and Cth cycle, and if dC = 1 cycle change,

$$R(C,Z) - R(C-1,Z) = k_1'S(C-1,Z) - k_2'R(C-1,Z) \qquad \text{(A-9)}$$

This is rearranged to give the recursive equation

$$R(C,Z) = k_1'S(C-1,Z) + (1-k_2')R(C-1,Z) \qquad \text{(A-10)}$$

If it is assumed that equilibrium has occurred during cycle C, then

$$\frac{R(C,Z)}{S(C,Z+1)} = \frac{\alpha}{\beta} = K \qquad \text{(A-11)}$$

where K is the distribution coefficient and $\alpha + \beta = 1$

But since

$$K = k_1'/k_2' \qquad \text{(A-12)}$$

and

$$k_1' + k_2' = \frac{k'}{k_1 + k_2} + \frac{k_2}{k_1 + k_2} = 1 \qquad \text{(A-13)}$$

then,

$$k_1' = \alpha = (1 - k_2') \qquad \text{(A-14)}$$

Thus,

$$R(C,Z) = \alpha[S(C-1,Z) + R(C-1,Z)] \qquad \text{(A-15)}$$

Using equation (A-11), the recursive equation for $S(C,Z+1)$ can be shown to be

$$S(C,Z+1) = \beta[S(C-1,Z) + R(C-1,Z)] \qquad \text{(A-16)}$$

The approach taken with ARDISC is that R and S are not equilibrated with each other in a given zone during a given cycle so that

$$\frac{R(C,Z)}{S(C,Z+1)} \neq \frac{\alpha}{\beta} \qquad \text{(A-17)}$$

To develop recursive equations for R and S for each zone and cycle, the following reaction can be established:

$$S^* \xoverleftarrow{*k_1'} S \underset{k_R'}{\overset{k_S'}{\rightleftarrows}} R \xrightarrow{*k_2'} R^*$$
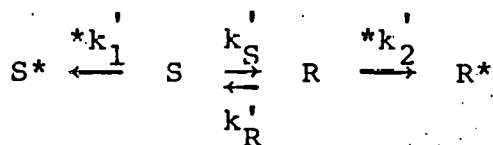
where, at the start of each cycle C,

$$R^*(C,Z) = S^*(C,Z) = 0 \qquad \text{(A-18)}$$

and at the end of each cycle C,

$$R(C,Z) = S(C,Z+1) = 0 \qquad \text{(A-19)}$$

The distinction between S* and S and between R* and R is an artificial one, made for the purpose of mathematically describing a partially equilibrated system using reactions which themselves go to equilibrium. With this description

$$\frac{dR}{dC} = -k_R'R + k_S'S \qquad \text{(A-20)}$$

and

$$\frac{dS}{dC} = -k_S' S + k_R' R \tag{A-21}$$

where

$$k_2' = k_R' + *k_2' \tag{A-22}$$

and

$$k_1' = k_S' + *k_1' \tag{A-23}$$

The rate constants k_1 and k_2 are the dimensionless rate constants discussed in earlier discussions of first order rate reactions.

If F and G are defined such that

$$F = \frac{k_S'}{k_S' + *k_1'} \tag{A-24}$$

$$G = \frac{k_R'}{k_R' + *k_2'} \tag{A-25}$$

equations (A-20) and (A-21) can be written

$$\left(\frac{dR}{dC}\right) = -Gk_2' R + Fk_1' S \tag{A-26}$$

$$\left(\frac{dS}{dC}\right) = -Fk_1' S + Gk_2' R \tag{A-27}$$

Again, letting dC = 1 cycle, these equations can be transformed:

$$R(C,Z) - R(C-1,Z) = -Fk_1' S(C-1,Z) + Gk_2' R(C,Z) \tag{A-28}$$

$$S(C,Z+1) - S(C-1,Z) = -Gk_2' R(C-1,Z) + Fk_1' S(C-1,Z) \tag{A-29}$$

or, upon rearranging and with $k_1 = \alpha$ and $k_2 = \beta$

$$R(C,Z) = [G\alpha-G+1]R(C-1,Z) + F\alpha S(C-1,Z) \qquad (A-30)$$

$$S(C,Z+1) = [F\beta-F+1]S(C-1,Z) + G\beta R(C-1,Z) \qquad (A-31)$$

These are the recursion equations used in the ARDISC model.

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