Appendix A
Linearity of Equations in SECO-TRANSPORT

The SECO-TRANSPORT calculations are linear with respect to the radionuclide source rate into the Culebra. Conceptually, SECO-TRANSPORT is solving a system of equations of the form

$$\mathbf{Du} = \mathbf{h}, \tag{A.1}$$

where $\mathbf{D}$ is a linear differential operator, $\mathbf{u}$ is radionuclide concentration, and $\mathbf{h}$ is the source rate into the system. If $\mathbf{u}_1$ and $\mathbf{u}_2$ are solutions to

$$\mathbf{Du}_1 = \mathbf{h}_1 \text{ and } \mathbf{Du}_2 = \mathbf{h}_2, \tag{A.2}$$

c_1 and c_2 are constants and $\mathbf{u} = c_1\mathbf{u}_1 + c_2\mathbf{u}_2$, then

$$\mathbf{Du} = \mathbf{D}(c_1\mathbf{u}_1 + c_2\mathbf{u}_2) = c_1\mathbf{Du}_1 + c_2\mathbf{Du}_2 = c_1\mathbf{h}_1 + c_2\mathbf{h}_2 \tag{A.3}$$

and thus $\mathbf{u}$ is a solution to

$$\mathbf{Du} = c_1\mathbf{h}_1 + c_2\mathbf{h}_2. \tag{A.4}$$

As a result, it is possible to solve the transport equations in SECO-TRANSPORT for a sequence of instantaneous unit releases to the Culebra and then use these results to construct the releases to the accessible environment that result from arbitrary time-dependent releases into the Culebra.

The implications of the linearity of Eq. (A.1) is perhaps best seen by formally examining the outcome of the numerical procedure used to obtain approximations to its solution. In SECO-TRANSPORT, Eq. (A.1) is solved with a finite difference procedure that is implicit in time over each time step. This procedure is based on dividing the time interval $[0, t_f]$ under consideration into a sequence of times $0 = t_0 < t_1 < \ldots, t_n = t_f$ and dividing the physical region (i.e., fracture and associated matrix) under consideration into a three dimensional grid of nodes as indicated in Fig. A.1. The approximate solution is then incremented from time t_{i-1} to time t_i by a relationship of the form

$$\mathbf{y}(t_i) = \mathbf{y}(t_{i-1}) + \mathbf{A}(t_{i-1}, t_i)\,\mathbf{y}(t_{i-1}) + \mathbf{B}(t_{i-1}, t_i)\,\mathbf{y}(t_i) + \mathbf{h}(t_{i-1}, t_i), \tag{A.5}$$

where

$\mathbf{y}(t)$ = vector of approximate solutions (i.e., at each node illustrated in Fig. A.1) at time t,

$\mathbf{h}(t_{i-1}, t_i)$ = vector of radionuclide inflows to the system over $[t_{i-1}, t_i]$,

$\mathbf{A}(t_{i-1}, t_i)$ = matrix associated with finite difference procedure for incrementing solution over $[t_{i-1}, t_i]$,

$\mathbf{B}(t_{i-1}, t_i)$ = matrix associated with finite difference procedure for incrementing solution over $[t_{i-1}, t_i]$.

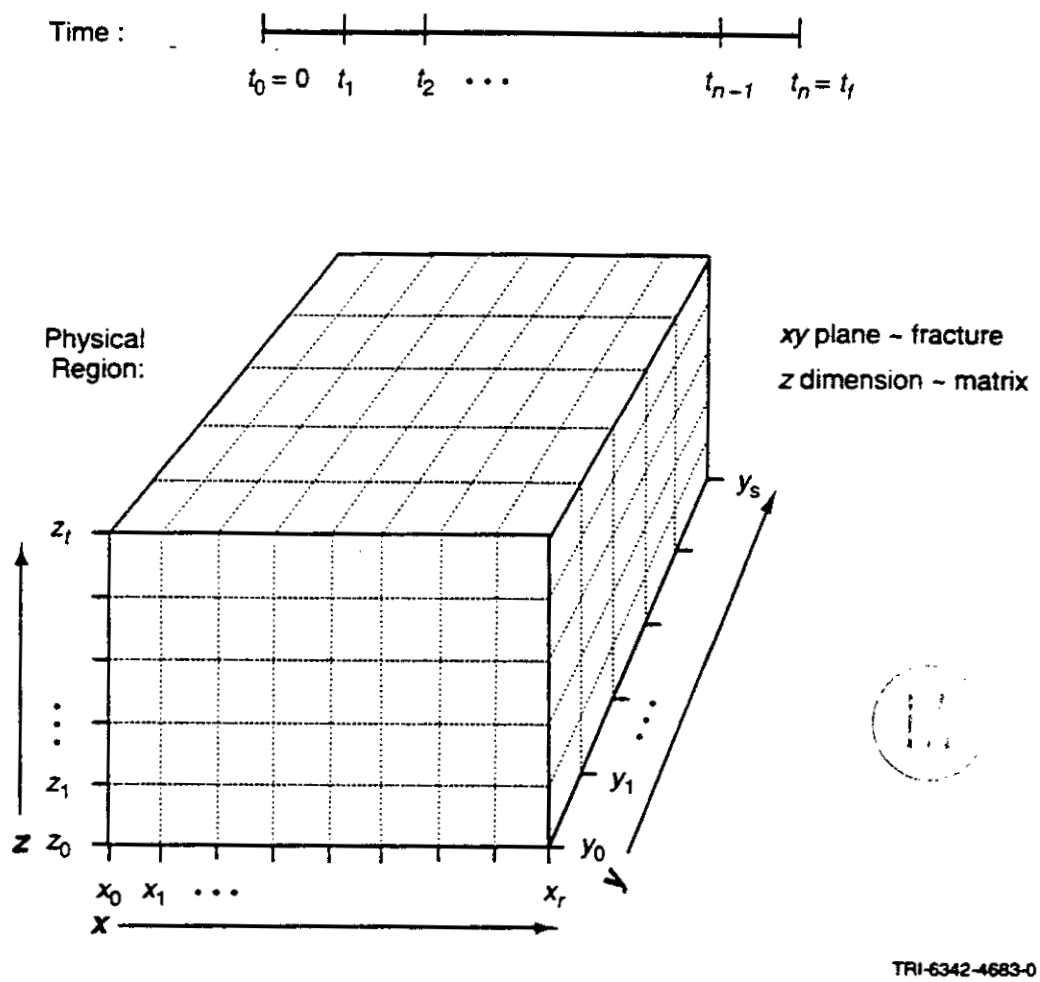

Figure A.1. Conceptual illustration of gridding used in finite difference procedure to solve the transport equations in SECO-TRANSPORT.

For notational convenience in later manipulations, the preceding relationships can be represented by

$$\mathbf{y}_t = \mathbf{y}_{t-1} + \mathbf{A}_t\mathbf{y}_{t-1} + \mathbf{B}_t\mathbf{y}_t + \mathbf{h}_t. \tag{A.6}$$

As an example, if 1000 nodes were used in the finite difference procedure, then $\mathbf{y}$ and $\mathbf{h}$ would be vectors from R^{1000}, and $\mathbf{A}$ and $\mathbf{B}$ would be 1000×1000 matrices. As radionuclide release to the system would occur over a relatively small area, most elements of $\mathbf{h}$ would be zero. Due to the nature of the numerical procedure, $\mathbf{A}$ and $\mathbf{B}$ would be banded matrices with most of their elements also equal to zero.

The numerical procedure indicated in Eqs. (A.5) and (A.6) leads to

$$(\mathbf{I}-\mathbf{B}_t)\mathbf{y}_t = (\mathbf{I}+\mathbf{A}_t)\mathbf{y}_{t-1} + \mathbf{h}_t \tag{A.7}$$

and thus to

$$\mathbf{y}_t = (\mathbf{I}-\mathbf{B}_t)^{-1}(\mathbf{I}+\mathbf{A}_t)\mathbf{y}_{t-1} + (\mathbf{I}-\mathbf{B}_t)^{-1}\mathbf{h}_t. \tag{A.8}$$

The nature of the solution to Eq. (A.1) can be seen by repetitively implementing the relationship in Eq. (A.8):

$$\mathbf{y}_1 = (\mathbf{I}-\mathbf{B}_1)^{-1}(\mathbf{I}+\mathbf{A}_1)\mathbf{y}_0 + (\mathbf{I}-\mathbf{B}_1)^{-1}\mathbf{h}_1 \tag{A.9}$$

$$\begin{aligned}\mathbf{y}_2 &= (\mathbf{I}-\mathbf{B}_2)^{-1}(\mathbf{I}+\mathbf{A}_2)\mathbf{y}_1 + (\mathbf{I}-\mathbf{B}_2)^{-1}\mathbf{h}_2 \\ &= (\mathbf{I}-\mathbf{B}_2)^{-1}(\mathbf{I}+\mathbf{A}_2)(\mathbf{I}-\mathbf{B}_1)^{-1}(\mathbf{I}+\mathbf{A}_1)\mathbf{y}_0 + (\mathbf{I}-\mathbf{B}_2)^{-1}(\mathbf{I}+\mathbf{A}_2)(\mathbf{I}-\mathbf{B}_1)^{-1}\mathbf{h}_1 + (\mathbf{I}-\mathbf{B}_2)^{-1}\mathbf{h}_2\end{aligned} \tag{A.10}$$

$$\begin{aligned}\mathbf{y}_3 &= (\mathbf{I}-\mathbf{B})^{-1}(\mathbf{I}+\mathbf{A}_3)\mathbf{y}_2 + \mathbf{I}(\mathbf{I}-\mathbf{B}_3)^{-1}\mathbf{h}_3 \\ &= \left[\prod_{j=3}^{1}(\mathbf{I}-\mathbf{B}_3)^{-1}(\mathbf{I}+\mathbf{A}_j)\right]\mathbf{y}_0 + \sum_{i=1}^{3}\left[\prod_{j=3}^{i+1}(\mathbf{I}-\mathbf{B}_j)^{-1}(\mathbf{I}+\mathbf{A}_j)\right](\mathbf{I}-\mathbf{B}_i)^{-1}\mathbf{h}_i\end{aligned} \tag{A.11}$$

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$$\begin{aligned}\mathbf{y}_n &= (\mathbf{I}-\mathbf{B}_n)^{-1}(\mathbf{I}+\mathbf{A}_n)\mathbf{y}_{n-1} + (\mathbf{I}-\mathbf{B}_n)^{-1}\mathbf{h}_n \\ &= \left[\prod_{j=n}^{1}(\mathbf{I}-\mathbf{B}_j)^{-1}(\mathbf{I}+\mathbf{A}_j)\right]\mathbf{y}_0 + \sum_{i=1}^{n}\left[\prod_{j=n}^{i+1}(\mathbf{I}-\mathbf{B}_j)^{-1}(\mathbf{I}+\mathbf{A}_j)\right](\mathbf{I}-\mathbf{B}_i)^{-1}\mathbf{h}_i\end{aligned} \tag{A.12}$$

with the identity

$$\prod_{j=n}^{nH}(\mathbf{I}-\mathbf{B}_j)^{-1}(\mathbf{I}+\mathbf{A}_j) = \mathbf{I} \tag{A.13}$$

being assumed for notational convenience.

As examination of the expression in Eq. (A.12) shows, it is possible to separate the part of the solution $\mathbf{y}_n$ that arises from the initial value condition $\mathbf{y}_0$ from the part that arises from the inflows to the system characterized by the $\mathbf{h}_i$. Further, similar terms appear in the parts of the solution associated with $\mathbf{y}_0$ and with the $\mathbf{h}_i$. Due to this repetition and the linearity of matrix multiplication, solutions to Eq. (A.1) for unit inputs to the system at fixed points in time can be used to construct the solutions that would result for an arbitrary function $\mathbf{h}$.

For convenience in discussion, assume that one or more of the elements of the vectors $\mathbf{y}_i$ appearing in Eq. (A.5) and in subsequent equations are used to accumulate integrated releases to the accessible environment and that a is a vector of 0's and 1's such that the total integrated release to the accessible environment through time t_i is given by $\mathbf{a}^T\mathbf{y}_i$. Further, assume that the numerical procedure indicated in Eq. (A.5) has been carried out to obtain

$\mathbf{y}_{u0j}$ = outcome of evaluating Eq. (A.5) through time t_j for a unit initial value $\mathbf{y}_{u0}$ at time t_0 (i.e., $\|\mathbf{y}_{u0}\| = 1$) and no other inputs to the system, (A.14)

$\mathbf{y}_{uij}$ = outcome of evaluating Eq. (A.5) through time t_j for the initial value $\mathbf{y}_0 = 0$, a unit input $\mathbf{h}_{ui}$ over the interval $[t_{j-1},t_j]$ (i.e., $\|\mathbf{h}_{ui}\| = 1$) and no other inputs to the system. (A.15)

As will be shown, $\mathbf{y}_{u0j}$ and $\mathbf{y}_{uij}$ can be used to construct solutions to Eq. (A.1) for initial values $\mathbf{y}_0$ and source rates $\mathbf{h}$ that can be obtained by scaling $\mathbf{y}_{u0}$ and $\mathbf{h}_{ui}$.

Suppose the initial value $\mathbf{y}_0$ and the source rate $\mathbf{h}(t)$ can be approximated by

$$\mathbf{y}_0 = c_0\mathbf{y}_{u0} \tag{A.16}$$

and

$$\int_{t_{i-1}}^{t_i} \mathbf{h}(t)dt = c_i\mathbf{h}_{ui}, \tag{A.17}$$

where the c_i, $i = 0, 1, \ldots, n$, are appropriately chosen constants. The integrated release $iR(t_n)$ to the accessible environment through time t_n associated with $\mathbf{y}_0$ and $\mathbf{h}$ can be approximated by

$$
\begin{aligned}
iR(t_n) &= \mathbf{a}^T \mathbf{y}_n \\
&= \mathbf{a}^T \left\{ \left[\prod_{j=n}^{1} (\mathbf{I} - \mathbf{B}_j)^{-1} (\mathbf{I} + \mathbf{A}_j) \right] \mathbf{y}_0 + \sum_{i=1}^{n} \left[\prod_{j=n}^{i+1} (\mathbf{I} - \mathbf{B}_j)^{-1} (\mathbf{I} + \mathbf{A}_j) \right] (\mathbf{I} - \mathbf{B}_i)^{-1} \mathbf{h}_i \right\} \\
&= \mathbf{a}^T \left\{ c_0 \left[\prod_{j=n}^{1} (\mathbf{I} - \mathbf{B}_j)^{-1} (\mathbf{I} + \mathbf{A}_j) \right] \mathbf{y}_{u0} + \sum_{i=1}^{n} c_i \left[\prod_{j=n}^{i+1} (\mathbf{I} - \mathbf{B}_j)^{-1} (\mathbf{I} + \mathbf{A}_j) \right] (\mathbf{I} - \mathbf{B}_i)^{-1} \mathbf{h}_{ui} \right\} \\
&= \mathbf{a}^T \left\{ c_0 \mathbf{y}_{u0n} + \sum_{i=1}^{n} c_i \mathbf{y}_{uin} \right\} \\
&= \sum_{i=0}^{n} c_i \mathbf{a}^T \mathbf{y}_{uin} \\
&= \sum_{i=0}^{n} c_i \; iR_u(t_i, t_n),
\end{aligned}
\tag{A-18}
$$

where

$$
\begin{aligned}
iR_u(t_i, t_n) &= \mathbf{a}^T \mathbf{y}_{uij} \\
&= \text{integrated release to accessible environment between } t_i \text{ and } t_n \text{ that results} \\
&\quad \text{from } \mathbf{y}_{u0} \text{ for } i = 0 \text{ and from } \mathbf{h}_{ui} \text{ for } i = 1, 2, \ldots, n.
\end{aligned}
\tag{A.19}
$$

Thus, by calculating and saving the integrated releases $iR_u(t_i, t_n)$, it is possible to calculate the integrated releases to the accessible environment for many different patterns of release to the Culebra (i.e., release functions $\mathbf{h}$) without repeating the numerical procedure required to solve Eq. (A.1).

The preceding computational strategy can also be used to estimate the release of a member of a decay chain to the accessible environment due to groundwater transport in the Culebra. In particular, if radionuclide k has $nP(k)$ precursors as indicated in Table A.1, $\mathbf{y}_{0l}$ and $\mathbf{h}_l(t)$ are the initial values and source rates associated with radionuclide k and its precursors for $l = k - nP(k), \ldots, k$, and $iR_k(t_n)$ is the integrated release of radionuclide k to the accessible environment through time t_n associated with the quantities $\mathbf{y}_{0l}$ and $\mathbf{h}_l(t)$, then

$$
iR_k(t_n) = \sum_{l=k-nP(k)}^{k} \sum_{i=0}^{n} c_{il} \; iR_{ukl}(t_i, t_n),
\tag{A.20}
$$

where

Table A.1. Radionuclides and Decay Chains Used for Transport Calculations in the Culebra Dolomite (adopted from Tables 7.3-1 and 7.3-2 of SAND92-0700/4).

Decay Chains	
(1)	Pu-240
(2)	Am-241 → Np-237→ U-233 → Th-229
(3)	U-234 → Th-230 → Ra-226
(4)	Pu-239

Individual Radionclides (nR = 9)			
Radionuclide	Integer Designator	Np(i)	Half Life (yr)
Pu-240	1	0	
Am-241	2	0	
Np-237	3	1	
U-233	4	2	
Th-229	5	3	
U-234	6	0	
Th-230	7	1	
Ra-226	8	2	
Pu-239	9	0	

$\mathbf{y}_{0ul}$ = unit initial value for radionuclide l,

$\mathbf{y}_{0l}$ = $c_{0l}\,\mathbf{y}_{0ul}$ (c_{0l} a constant),

$\mathbf{h}_{uil}$ = unit input of radionuclide l over $[t_{i-1}, t_i]$,

$\int_{t_{i-1}}^{t_i} \mathbf{h}_l(t)dt = c_{il}\mathbf{h}_{uil}$ (c_{il} a constant),

$iR_{ukl}(t_0, t_n)$ = integrated release of radionuclide k to accessible environment between t_0 and t_n due to initial value $\mathbf{y}_{0ul}$ of radionuclide l,

$iR_{ukl}(t_i, t_n)$ = integrated release of radionuclide k to accessible environment between t_i and t_n due to release $\mathbf{h}_{uil}$ of radionuclide l, during $[t_{i-1}, t_i]$.

The expression in Eq. (A.20) can be established by following a sequence of manipulations analogous to those that lead to Eq. (A.18)

If the Culebra flow field obtained from SECO-FLOW is time-dependent, then it will be necessary to obtain the integrated releases $iR_u\left(t_i, t_n\right)$ in Eq. (A.19) from h_{ui} for $i = 1, 2, \ldots, n$. However, if the flow field is not time-dependent, then it will be necessary to solve Eq. (A.1) only for the initial value condition $\mathbf{y}_{u0}$ to obtain

$$iR_u\left(t_0, t_j\right), \; j = 1, 2, \ldots, n, \tag{A.21}$$

where $iR_u\left(t_0, t_j\right)$ is the integrated release to the accessible environment between t_0 and t_j that results from $\mathbf{y}_{u0}$. Then,

$$iR_u\left(t_i, t_n\right) = iR_u\left(t_0, t_{n-i}\right), \; i = 1, 2, \ldots, n, \tag{A.22}$$

due to the constancy of the flow field (i.e., a unit release at time t_j will transport in exactly the same manner as a unit release at time $t_0 = 0$. At present, it is anticipated that the 1996 WIPP PA will use constant (i.e., time invariant) flow fields in the Culebra.