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# APPROXIMATE SOLUTIONS FOR DIFFUSIONAL RELEASE FROM SALTSTONE VAULTS

**G. P. Flach**

**FEBRUARY 2009**

Savannah River National Laboratory
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Aiken, SC 29808

**Prepared for the U.S. Department of Energy Under Contract Number DE-AC09-08SR22470**

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## REVIEWS AND APPROVALS

2/26/09

Greg Flach, Author, Geo-Modeling Date

3/9/09

Glenn Taylor, Peer Reviewer, Radiological Performance Assessment Date

3/13/09

Heather Burns, Program Manager, Radiological Performance Assessment Date

3/10/09

Jack Mayer, Manager, Geo-Modeling Date

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## Introduction

A Saltstone vault is designed to perform as a low permeability barrier around Saltstone waste, such that diffusion controls contaminant release to surrounding soil. At later times the physical state of the vault may become sufficiently degraded that advection dominates transport.

An approximate, closed-form, analytic solution for diffusional release at early times, prior to extensive vault degradation, is desirable for GoldSim probabilistic analysis for computational efficiency. Also needed is an estimate of the contaminant mass that has diffused into the vault concrete prior to any hydraulic failure. Mass residing in the vault concrete at the time of failure is available for advective flushing and release.

## Heat Transfer - Mass Transfer Analogy

The equations describing heat conduction and mass diffusion are mathematically identical, differing only in the symbols and terminology conventionally associated with each application. Thus analytic solutions to heat conduction problems can be readily adapted to mass diffusion. The analogy between heat and mass diffusion is evident from a comparison of governing and flux equations for a non-sorbing, non-decaying, species:

| Heat Transfer (Myers, 1971) | Mass Transfer (de Marsily, 1986) | |
|---|---|---|
| $\frac{\partial t}{\partial \theta} = \alpha \frac{\partial^2 t}{\partial x^2}$ | $\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2}$ | (1a,b) |
| $q = -k \frac{\partial t}{\partial \theta}$ | $f = -nD \frac{\partial c}{\partial x}$ | (2a,b) |
| t = temperature | c = concentration | |
| θ = time | t = time | |
| x = length | x = length | |
| α = k/pc = thermal diffusivity | D = effective diffusion coefficient | |
| k = thermal conductivity | n = porosity | |
| ρc = heat capacity | f = mass flux | |
| q = heat flux | | |

The heat transfer equations describe heat conduction in a homogeneous, non-porous, medium. The mass transfer equation set describes mass diffusion in a homogeneous, porous, medium. The analogy between material properties is

$$k \leftrightarrow nD$$
$$\rho c \leftrightarrow n$$
$$\alpha \leftrightarrow D$$

The heat and mass transfer analogy can be used to derive the solution to a mass transfer problem from an existing heat transfer solution.

## Analytic Solutions for a Steady-State Transport

For example, consider steady-state heat conduction across a distance L. The flux of heat or mass is given by

| Heat Transfer | Mass Transfer | |
|---|---|---|
| $q = \frac{kt_0}{L}$ | $f = \frac{nDc_0}{L}$ by analogy | (3a,b) |
| q = heat flux<br>$t_0$ = temperature (difference)<br>k = thermal conductivity<br>L = length | f = mass flux<br>$c_0$ = concentration (difference)<br>n = porosity<br>D = effective diffusion coefficient<br>L = length | |

These and other analytical solutions are relevant to the Saltstone vault.

## Analytic Solutions for a Semi-Infinite Region

The Saltstone monolith is sufficiently large that it can be treated locally as a semi-infinite domain over the time period for which diffusion dominates transport. That is, ignoring corner effects, diffusional release through the roof, wall, and floor surfaces can be approximated as one-dimensional diffusion through a semi-infinite region.

For a homogeneous region with a uniform initial value (temperature or concentration), the corresponding heat and mass transfer solutions are

| Heat Transfer | Mass Transfer | | |
|---|---|---|---|
| $t = t_0 \mathrm{erfc}\left(\frac{x}{2\sqrt{\alpha\theta}}\right)$ | $c = c_0 \mathrm{erfc}\left(\frac{x}{2\sqrt{Dt}}\right)$ | value | (4a,b) |
| Myers (1971, eqn 6.4.29) | by analogy | | |
| $q = \frac{kt_0}{\sqrt{\pi\alpha\theta}} \exp\left(\frac{-x^2}{4\alpha\theta}\right)$ | $f = nc_0\sqrt{\frac{D}{\pi t}} \exp\left(\frac{-x^2}{4Dt}\right)$ | flux | (5a,b) |
| Myers (1971, cf. eqn 6.4.35) | by analogy | | |

These solutions are *generally* not directly applicable to the Saltstone system, which is a composite of vault concrete and Saltstone grout with differing properties. Furthermore, the initial value is zero in the vault concrete and non-zero in Saltstone grout (Figure 1). However, an exception occurs at long times, after the diffusion front has deeply penetrated the Saltstone material, when the effect of the thin concrete "skin" can be neglected. Another exception is leaching from both surfaces of a macroscopic crack through Saltstone grout.

Another analytic solution with relevance to Saltstone is the initial interface value of two contacting surfaces (Myers, 1971, Figure 6-9). The contact value is a function of the initial values and properties of the two materials (denoted by subscripts 0 and 1 on properties):

| Heat Transfer | Mass Transfer | |
|---|---|---|
| $t_i = \dfrac{t_0\sqrt{(k\rho c)_0} + t_1\sqrt{(k\rho c)_1}}{\sqrt{(k\rho c)_0} + \sqrt{(k\rho c)_1}}$ | $c_i = \dfrac{c_0 n_0\sqrt{D_0} + c_1 n_1\sqrt{D_1}}{n_0\sqrt{D_0} + n_1\sqrt{D_1}}$ | (6a,b) |
| Myers (1971, eqn 6.4.37) | by analogy | |
| $t_i$ = interface/contact temperature | $c_i$ = interface/contact concentration | |

$c_0$ is the concentration difference in Equation (3b). The interface value $c_i$ is time invariant.

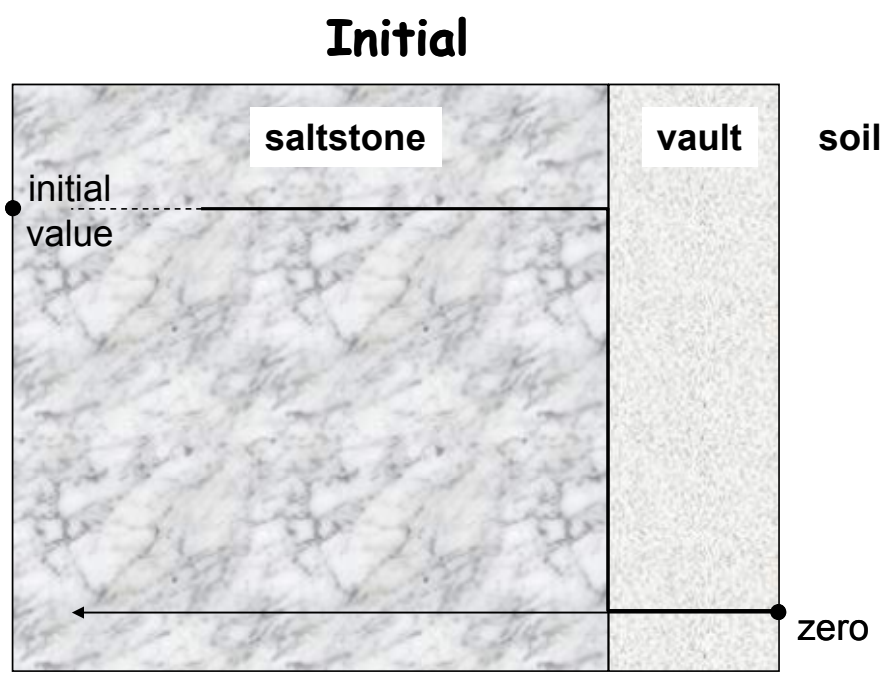


**Figure 1 – Initial conditions in Saltstone vault**

## Application to Saltstone

Figures 2 through 4 illustrate three conceptual stages of diffusional release from Saltstone, starting from the initial condition depicted in Figure 1. When contaminant bearing Saltstone is brought into contact with clean vault concrete, an interface concentration is established per Equation (6b). In the short term (Figure 2), diffusion occurs primarily in the immediate

vicinity of the contact interface. Equations (4b) and (5b), using vault concrete properties and the interface concentration from Equation (6b), define concentration and flux in the vault concrete:

$$f_{ST} = n_v c_i \sqrt{\frac{D_v}{\pi t}} \exp\left(\frac{-x^2}{4D_v t}\right) \tag{7a}$$

$$c_i = c_S \frac{n_S \sqrt{D_S}}{n_S \sqrt{D_S} + n_v \sqrt{D_v}} \tag{7b}$$

Here "v" and "S" denote the vault concrete and Saltstone grout. At intermediate times (Figure 3), the semi-infinite solution is no longer accurate, because the diffusion front has reached the outside surface of the vault. During this period, while the interface concentration is still near its initial value, the steady-state solution indicated by Equation (3b) is a reasonable surrogate. The initial interface concentration from Equation (7b) and vault concrete properties should be used:

$$f_{IT} = \frac{n_v D_v c_i}{L} \tag{8}$$

Long term, after the diffusion front penetrating Saltstone is deep compared to the concrete thickness, Equation (5b) using Saltstone properties and the initial Saltstone concentration would approximate the diffusional release:

$$f_{LT} = n_S c_S \sqrt{\frac{D_S}{\pi t}} \exp\left(\frac{-x^2}{4D_S t}\right) \tag{9}$$

A smoothly varying flux curve over the whole time domain is desirable. This objective can be accomplished by blending the short and long term solutions, and checking for consistency with the intermediate flux estimate. The relative concentration at the outside vault surface computed from Equation (4b) varies between 0 and 1 over the intermediate time frame, and is a reasonable candidate for a weighting function. With this assumption, the composite flux becomes

$$f = \exp\left[\left(1 - \frac{c_L}{c_i}\right) \ln f_{ST} + \left(\frac{c_L}{c_i}\right) \ln f_{LT}\right] \tag{10}$$

where blending is done in logarithm-space, analogous to geometric averaging. The intermediate time flux expression is used only as a point of reference. The relative concentration is defined by

$$\frac{c_L}{c_i} = \mathrm{erfc}\left(\frac{L}{2\sqrt{D_v t}}\right) \tag{11}$$

where L is the vault thickness.

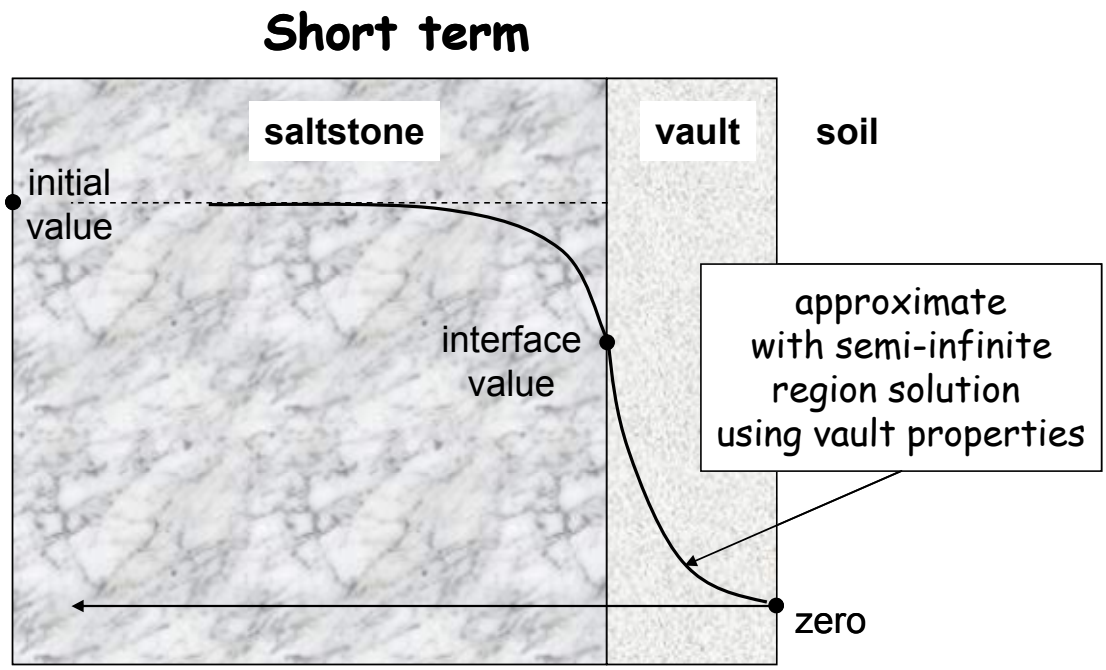


**Figure 2 – Short-term concentration profile.**

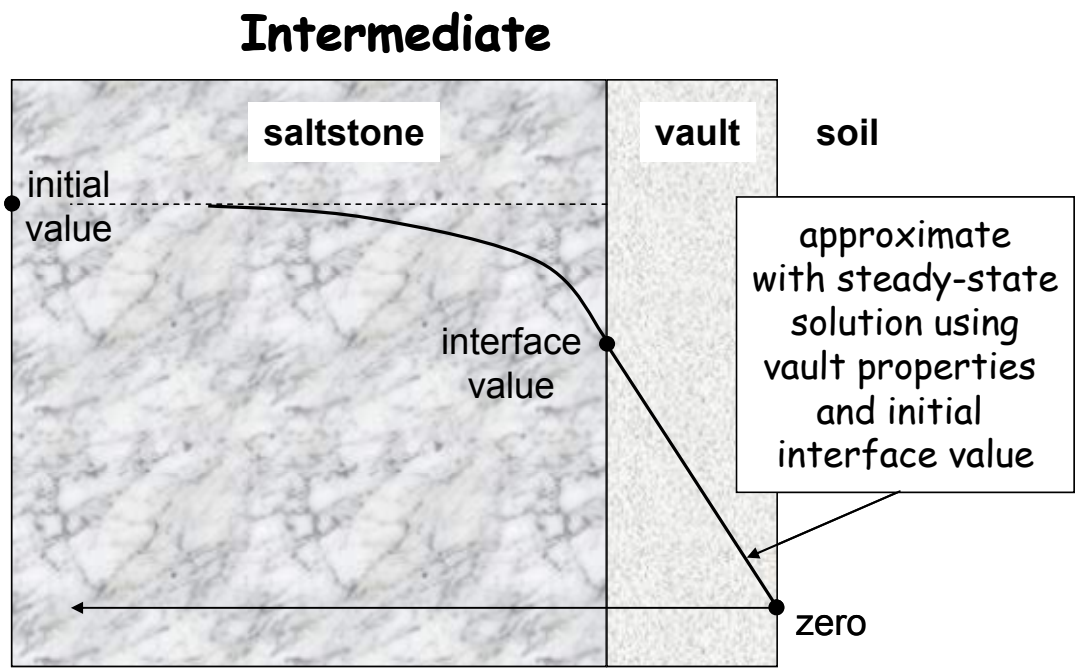


**Figure 3 – Intermediate concentration profile**

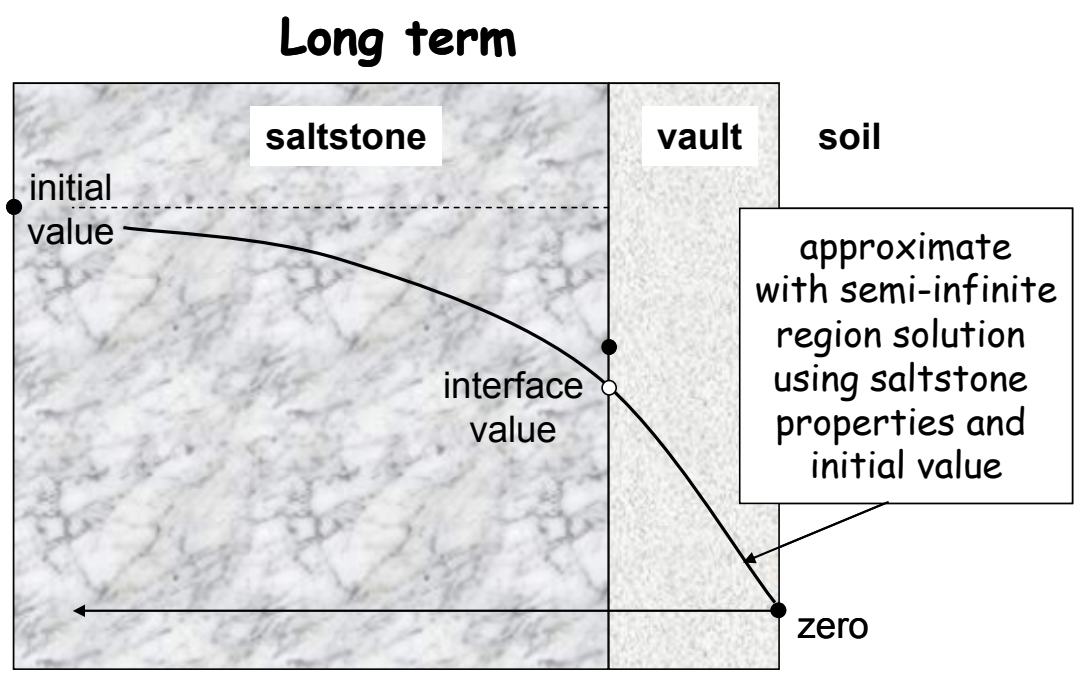


**Figure 4 – Long-term concentration profile**

## Extension to Decaying and Sorbing Species

The governing equation defining diffusion of a decaying and sorbing species is

$$\frac{\partial c}{\partial t} = D_R \frac{\partial^2 c}{\partial x^2} - \lambda c \tag{12}$$

where

$D_R = \frac{D}{R}$ = retarded diffusion coefficient

$R = 1 + \frac{(1-n)\rho_s K_d}{n}$ = retardation factor

$K_d$ = soil-solute distribution coefficient

$\lambda = \frac{\ln 2}{\tau}$ = first-order decay constant

$\tau$ = half-life

and the other symbols are as defined earlier. The impact of linear sorption is simply a modified effective diffusion coefficient, which retards the rate of diffusion. Radioactive decay introduces a new first-order sink term.

Transport of a decaying species can be related to that of a non-decaying species through a simple transformation. Consider mass diffusion from a semi-infinite domain with a uniform initial concentration equal to 1 (without loss of generality). A complete equation set, including initial and boundary conditions, is

$$\frac{\partial c}{\partial t} = D_R \frac{\partial^2 c}{\partial x^2} - \lambda c \tag{13a}$$

$$c(0,t) = 0 \tag{13b}$$

$$c(\infty,t) = \exp(-\lambda t) \tag{13c}$$

$$c(x,0) = 1 \tag{13d}$$

A reasonable hypothesis is that concentration can be decomposed as the product

$$c = \exp(-\lambda t) \cdot c^*(x,t) \tag{14}$$

where $c^*$ is the undefined transformed concentration. By substitution of Equation (14) into Equations (13), the transformed concentration is shown to satisfy the following equation set

$$\frac{\partial c^*}{\partial t} = D_R \frac{\partial^2 c^*}{\partial x^2} \tag{15a}$$

$$c^*(0,t) = 0 \tag{15b}$$

$$c^*(\infty,t) = 1 \tag{15c}$$

$$c^*(x,0) = 1 \tag{15d}$$

Thus $c^*$ is recognized as the solution for a non-decaying species, and the solution for a decaying species is gotten by multiplying by $\exp(-\lambda t)$.

The flux for a decaying and sorbing species is computed as

$$\begin{aligned} f &= -nD\frac{\partial c}{\partial x} \\ &= -nD\frac{\partial c^*}{\partial x}\cdot\exp(-\lambda t) \\ &= -nD_R\frac{\partial c^*}{\partial x}\cdot R\cdot\exp(-\lambda t) \\ &= f^*(D_R)\cdot R\cdot\exp(-\lambda t) \end{aligned} \tag{16}$$

which is recognized as the flux expression for a non-decaying and non-sorbing species ($f^*$) evaluated with $D_R$ (instead of D), multiplied by retardation factor R and $\exp(-\lambda t)$.

## Mass in vault thickness

Should the vault fail hydraulically, any contaminant residing in the vault would be available for release by advective flushing. For this situation an estimate of total contaminant mass, in solution and sorbed to solids, is needed to define the inventory prior to advective release. The mass of solute in the Saltstone vault thickness is given by

$$M(t) = n\int_0^L c(x,t)dx \tag{17}$$

where L is the vault thickness, and n is the vault porosity. In the short term, the concentration is defined by Equation (4b), using the interface concentration and vault concrete properties

$$c = c_i \operatorname{erfc}\left(\frac{x}{2\sqrt{Dt}}\right) \tag{18}$$

Substituting Equation (18) into Equation (17) yields

$$M_{ST}(t) = nc_i \int_0^L \operatorname{erfc}\left(\frac{x}{2\sqrt{Dt}}\right) dx \tag{19}$$

The indefinite integral of the complementary error function is given by Mathematica documentation as (http://functions.wolfram.com/GammaBetaErf/Erfc/21/01/01/)

$$\int \operatorname{erfc}(a\,z)\,dz = z\operatorname{erfc}(a\,z) - \frac{e^{-a^2 z^2}}{a\sqrt{\pi}} \tag{20}$$

Integration of Equation (19) produces

$$\begin{aligned} M_{ST}(t) &= nc_i \left[ x \cdot \operatorname{erfc}\left(\frac{x}{2\sqrt{Dt}}\right) - \frac{\exp\left(-\frac{x^2}{4Dt}\right)}{\frac{1}{2\sqrt{Dt}}\sqrt{\pi}} \right]_0^L \\ &= nc_i \left[ x \cdot \operatorname{erfc}\left(\frac{x}{2\sqrt{Dt}}\right) - \frac{2\sqrt{Dt}}{\sqrt{\pi}} \exp\left(-\frac{x^2}{4Dt}\right) \right]_0^L \\ &= nc_i \left[ L \cdot \operatorname{erfc}\left(\frac{L}{2\sqrt{Dt}}\right) - \frac{2\sqrt{Dt}}{\sqrt{\pi}} \exp\left(-\frac{L^2}{4Dt}\right) + \frac{2\sqrt{Dt}}{\sqrt{\pi}} \right] \\ &= nc_i \left\{ L \cdot \operatorname{erfc}\left(\frac{L}{2\sqrt{Dt}}\right) + \frac{2\sqrt{Dt}}{\sqrt{\pi}} \left[ 1 - \exp\left(-\frac{L^2}{4Dt}\right) \right] \right\} \end{aligned} \tag{21}$$

The long term solution for mass proceeds in a similar, but differing manner. The concentration expression involves the error function instead of the complementary error function in Equation (18):

$$c = c_0 \operatorname{erf}\left(\frac{x}{2\sqrt{D_S t}}\right) \tag{22}$$

The solution is referenced to the initial Saltstone concentration, and uses Saltstone properties (denoted explicitly by the "S" subscript). The indefinite integral of the error function is given by Mathematica documentation as
(http://functions.wolfram.com/GammaBetaErf/Erfc/21/01/01/)

$$\int \operatorname{erf}(a\,z)\,dz == z\,\operatorname{erf}(a\,z) + \frac{e^{-a^2 z^2}}{a\sqrt{\pi}} \tag{23}$$

Integration of Equation (17) using Equations (22) and (23) yields the following expression for long-term solute mass

$$M_{LT}(t) = n_v c_0 \left\{ L \cdot \operatorname{erf}\left( \frac{L}{2\sqrt{D_S t}} \right) - \frac{2\sqrt{D_S t}}{\sqrt{\pi}} \left[ 1 - \exp\left( -\frac{L^2}{4 D_S t} \right) \right] \right\} \tag{24}$$

The porosity is that of the vault, now denoted explicitly with a "v" subscript.

Analogous to flux, the vault mass solutions for short and long term conditions can be blended following Equation (10):

$$M = \exp\left[ \left( 1 - \frac{c_L}{c_i} \right) \ln M_{ST} + \left( \frac{c_L}{c_i} \right) \ln M_{LT} \right] \tag{25}$$

For sorbing species, the total mass present in the vault thickness is

$$M_T = M \cdot R \tag{26}$$

where R is the retardation coefficient of vault defined earlier. For a sorbing and decaying species, the mass is reduced by $\exp(-\lambda t)$ resulting in the general expression

$$M_T = M \cdot R \cdot \exp(-\lambda t) \tag{27}$$

## Representative calculations

Figure 5 illustrates the diffusion flux predicted for the set of parameters presented in the Appendix A, in particular an 8 inch concrete vault in contact with Saltstone. The predicted flux, obtained by blending the short- and long-term solutions, peaks slightly above the intermediate flux reference. The latter suggests a modest over-prediction, which would tend to be conservative.

Figures 6a-d show the release predicted for the a) no sorption and no decay, b) sorption but no decay, c) decay but no sorption, and d) sorption and decay. Figure 6a is the same as Figure 5, except for the vertical scale. Figure 7 shows example vault mass results for the same parameters varied in Figure 6. These figures also show PORFLOW numerical simulation results (gray line) for validation purposes. Additional flux and mass results, for Kd = 30, 300, and 3000 mL/g, are shown in Figures 8-10.

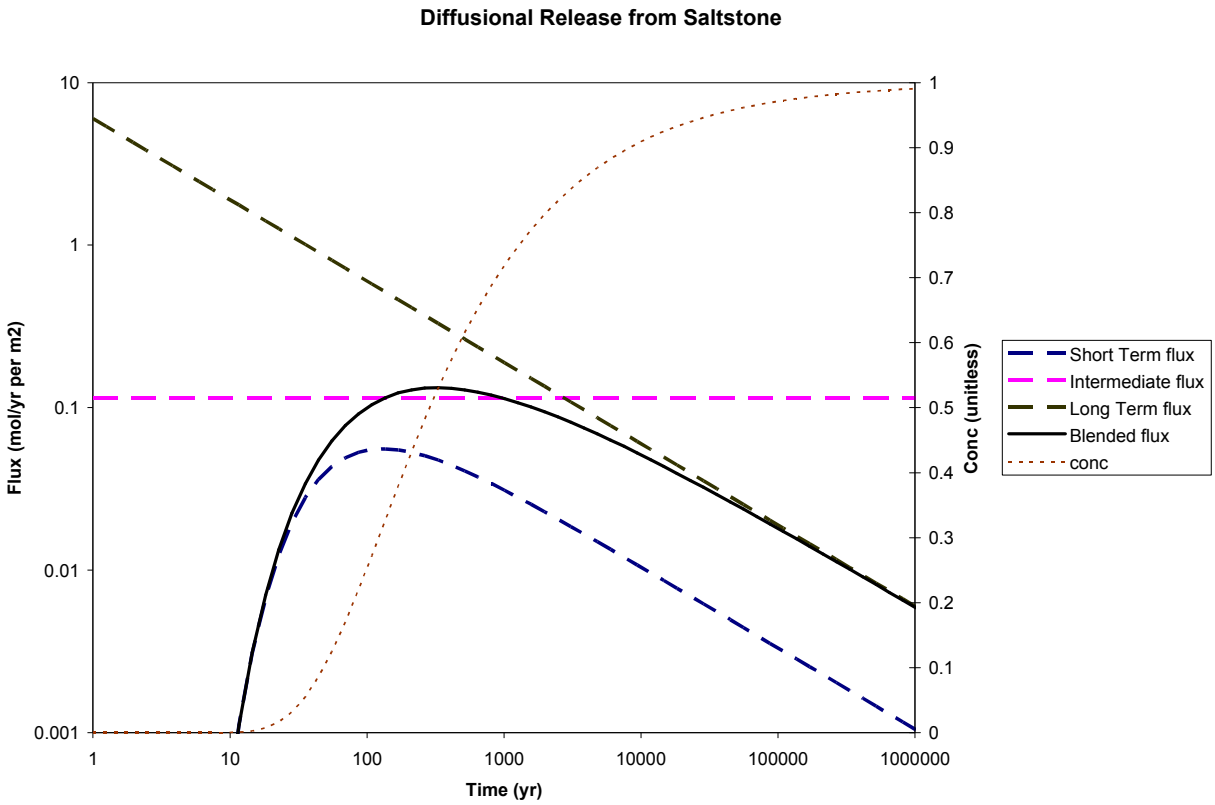


**Figure 5 – Diffusional release from Saltstone for an 8" Vault Thickness**

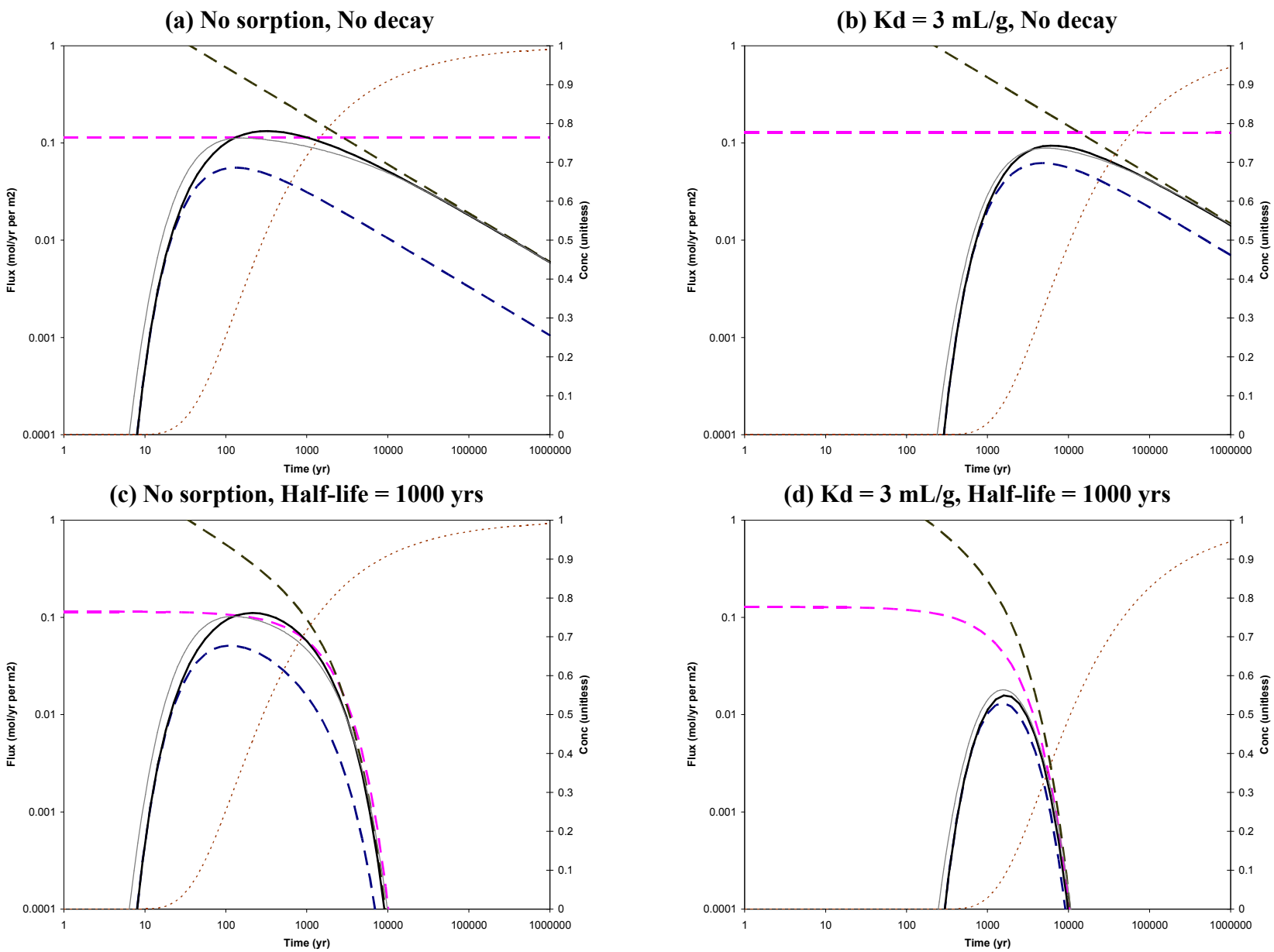


**Figure 6 - Parametric study involving decay and sorption; vault flux results**

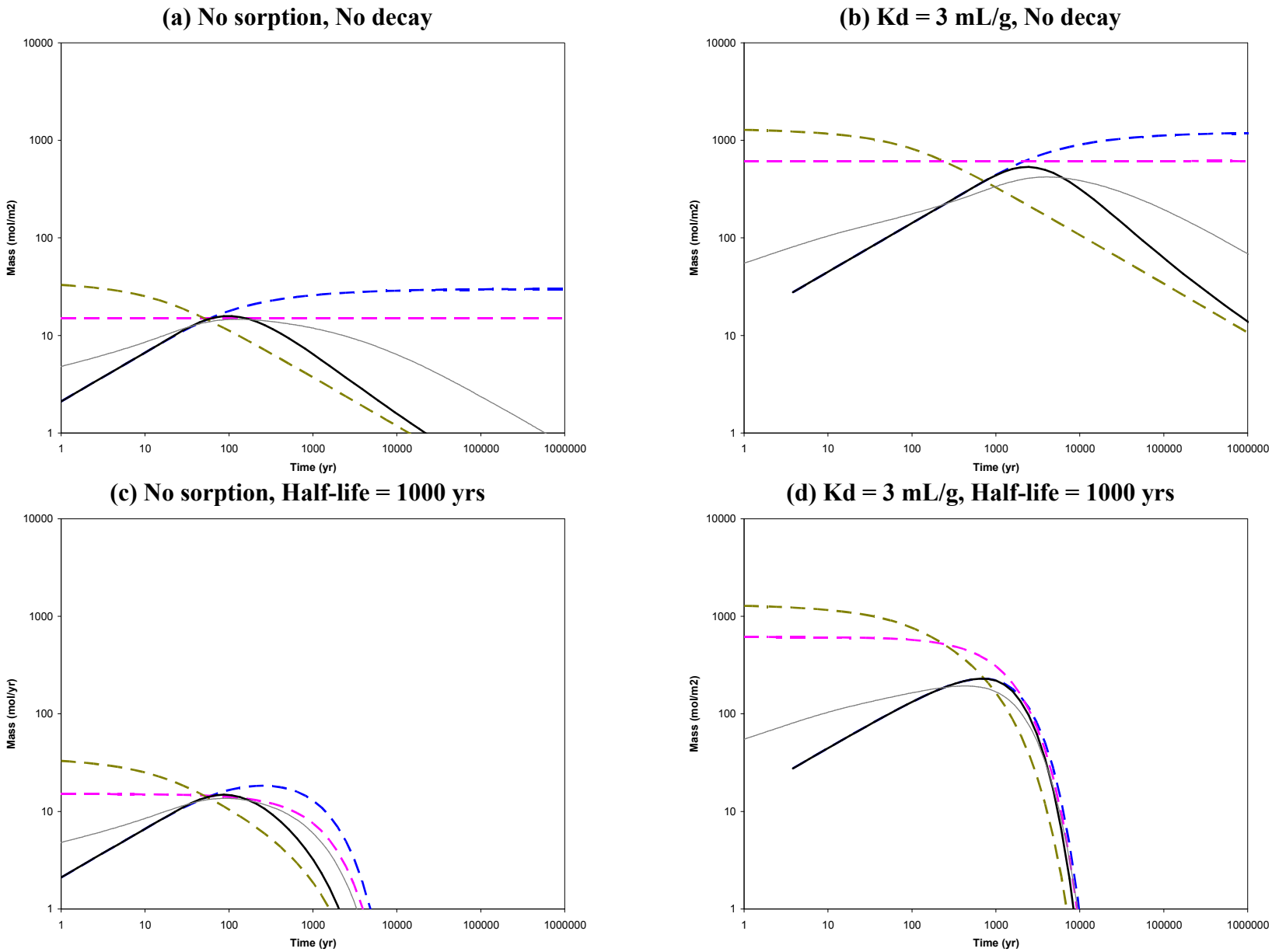


**Figure 7 - Parametric study involving decay and sorption; vault mass results.**

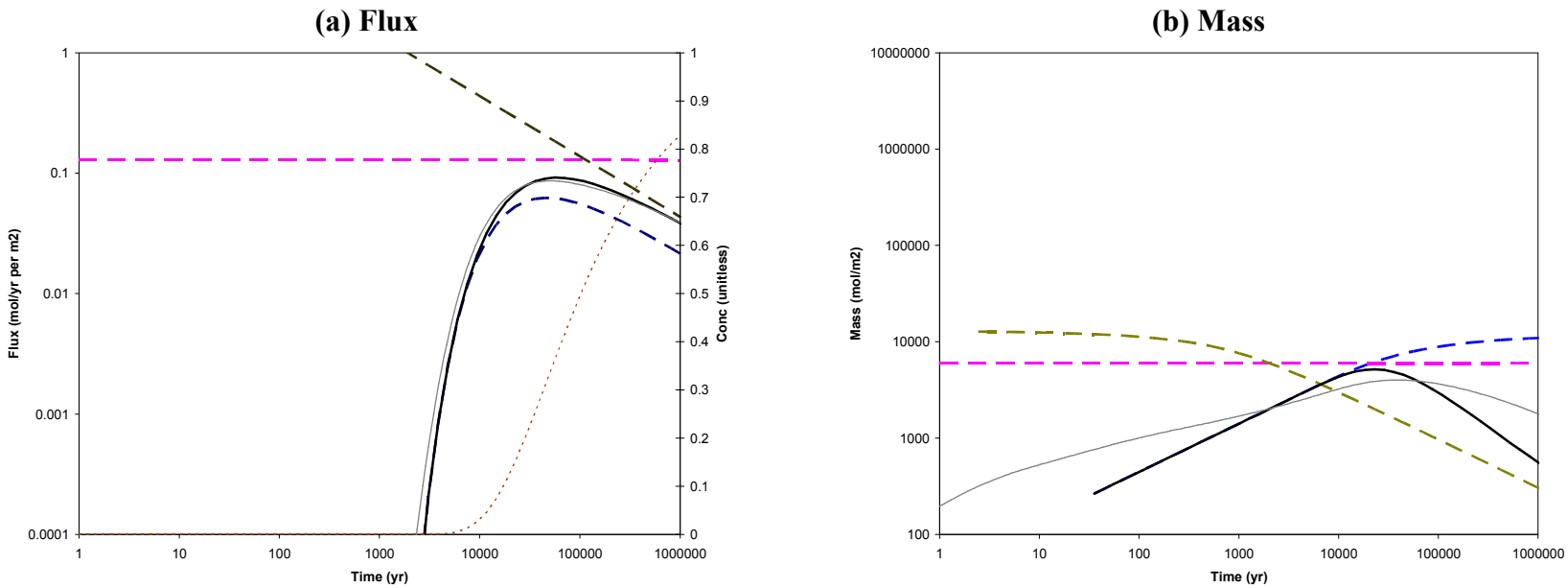


**Figure 8 - Flux and mass for Kd = 30 mL/g**

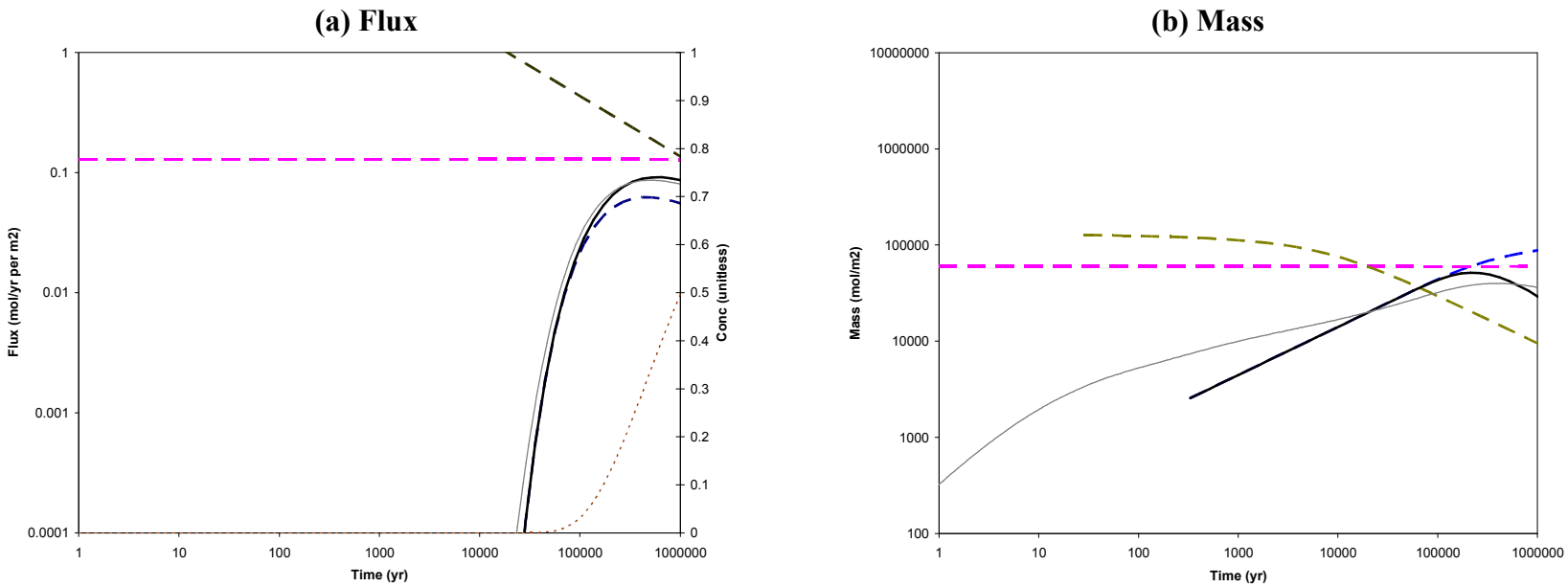


**Figure 9 - Flux and mass for Kd = 300 mL/g**

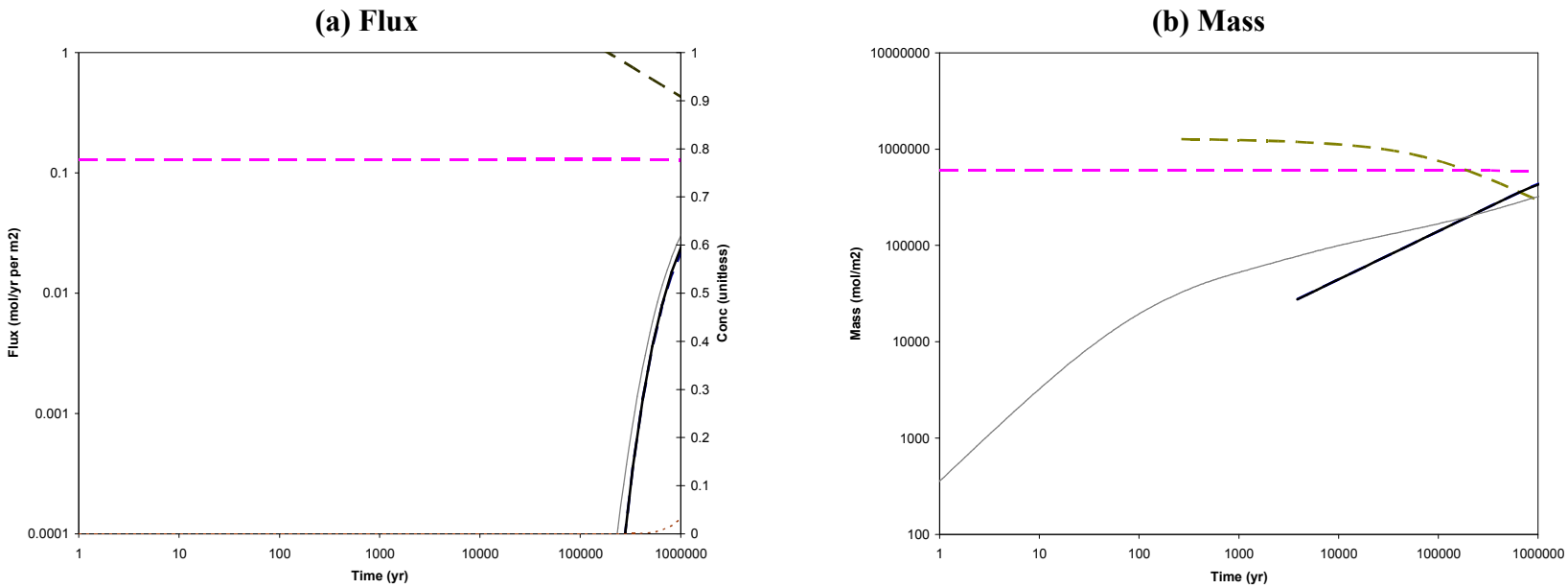


**Figure 10 - Flux and mass for Kd = 3000 mL/g**

## Acknowledgement

Ken Dixon (SRNL) generated the PORFLOW numerical results used to validate the approximate analytic predictions.

## References

Myers, G. E., 1971, Analytical Methods in Conduction Heat Transfer, McGraw-Hill, New York.

de Marsily, G., 1986, Quantitative Hydrogeology, Academic Press, Orlando.

# Appendix A - Parameters and calculations underlying Figures 5 and 6a

| | | |
|---|---|---|
| **Saltstone grout** | | |
| initial concentration, c | 1 | mol/L |
| porosity, n | 0.6 | unitless |
| effective diffusion coefficient, D | 1.0E-07 | $cm^2/s$ |
| n√D | 1.90E-04 | cm/√s |
| **Vault concrete** | | |
| initial concentration, c | 0 | mol/L |
| porosity, n | 0.18 | unitless |
| effective diffusion coefficient, D | 5.0E-08 | $cm^2/s$ |
| n√D | 4.02E-05 | cm/√s |
| **Interface** | | |
| concentration, c | **0.825** | mol/L |
| **Flux** | | |
| area, A | 1 | $m^2$ |
| | 10000 | $cm^2$ |
| thickness, x | 8 | in |
| | 20.3 | cm |
| time factor | 1.25 | |
| concentration, c | 0.825 | mol/L |
| | 0.000825 | $mol/cm^3$ |
| effective diffusion coefficient, D | 5.0E-08 | $cm^2/s$ |
| | 1.58 | $cm^2/yr$ |
| steady-state flux | 1.15E-01 | |
| concentration, c | 1.000 | mol/L |
| | 0.001 | $mol/cm^3$ |
| effective diffusion coefficient, D | 1.0E-07 | $cm^2/s$ |
| | 3.15 | $cm^2/yr$ |

| time | Short Term flux | Intermediate flux | conc | Long Term flux | Blended flux | Short Term mass | Intermediate mass | Long Term mass | Blended mass |
|---|---|---|---|---|---|---|---|---|---|
| yr | mol/yr | mol/yr | | mol/yr | mol/yr | mol | mol | mol | mol |
| 0.00E+00 | | | | | | | | | |
| 1.00E+00 | 3.9E-29 | 1.15E-01 | 0.00E+00 | 6.0E+00 | 3.9E-29 | 2.1E+00 | 1.5E+01 | 3.3E+01 | 2.1E+00 |
| 1.25E+00 | 1.7E-23 | 1.15E-01 | 0.00E+00 | 5.4E+00 | 1.7E-23 | 2.4E+00 | 1.5E+01 | 3.3E+01 | 2.4E+00 |
| 1.56E+00 | 5.4E-19 | 1.15E-01 | 0.00E+00 | 4.8E+00 | 5.4E-19 | 2.6E+00 | 1.5E+01 | 3.2E+01 | 2.6E+00 |
| 1.95E+00 | 2.1E-15 | 1.15E-01 | 2.22E-16 | 4.3E+00 | 2.1E-15 | 2.9E+00 | 1.5E+01 | 3.2E+01 | 2.9E+00 |
| 2.44E+00 | 1.5E-12 | 1.15E-01 | 2.42E-13 | 3.8E+00 | 1.5E-12 | 3.3E+00 | 1.5E+01 | 3.1E+01 | 3.3E+00 |
| 3.05E+00 | 2.9E-10 | 1.15E-01 | 5.75E-11 | 3.4E+00 | 2.9E-10 | 3.7E+00 | 1.5E+01 | 3.0E+01 | 3.7E+00 |
| 3.81E+00 | 1.9E-08 | 1.15E-01 | 4.67E-09 | 3.1E+00 | 1.9E-08 | 4.1E+00 | 1.5E+01 | 3.0E+01 | 4.1E+00 |
| 4.77E+00 | 5.3E-07 | 1.15E-01 | 1.61E-07 | 2.8E+00 | 5.3E-07 | 4.6E+00 | 1.5E+01 | 2.9E+01 | 4.6E+00 |
| 5.96E+00 | 7.3E-06 | 1.15E-01 | 2.77E-06 | 2.5E+00 | 7.3E-06 | 5.1E+00 | 1.5E+01 | 2.8E+01 | 5.1E+00 |
| 7.45E+00 | 5.9E-05 | 1.15E-01 | 2.76E-05 | 2.2E+00 | 5.9E-05 | 5.7E+00 | 1.5E+01 | 2.7E+01 | 5.7E+00 |
| 9.31E+00 | 3.1E-04 | 1.15E-01 | 1.77E-04 | 2.0E+00 | 3.1E-04 | 6.4E+00 | 1.5E+01 | 2.6E+01 | 6.4E+00 |
| 1.16E+01 | 1.1E-03 | 1.15E-01 | 7.98E-04 | 1.8E+00 | 1.1E-03 | 7.2E+00 | 1.5E+01 | 2.4E+01 | 7.2E+00 |
| 1.46E+01 | 3.1E-03 | 1.15E-01 | 2.70E-03 | 1.6E+00 | 3.1E-03 | 8.0E+00 | 1.5E+01 | 2.3E+01 | 8.0E+00 |
| 1.82E+01 | 6.7E-03 | 1.15E-01 | 7.30E-03 | 1.4E+00 | 7.0E-03 | 8.9E+00 | 1.5E+01 | 2.2E+01 | 9.0E+00 |
| 2.27E+01 | 1.2E-02 | 1.15E-01 | 1.64E-02 | 1.3E+00 | 1.3E-02 | 1.0E+01 | 1.5E+01 | 2.0E+01 | 1.0E+01 |
| 2.84E+01 | 2.0E-02 | 1.15E-01 | 3.18E-02 | 1.1E+00 | 2.2E-02 | 1.1E+01 | 1.5E+01 | 1.9E+01 | 1.1E+01 |
| 3.55E+01 | 2.8E-02 | 1.15E-01 | 5.49E-02 | 1.0E+00 | 3.4E-02 | 1.2E+01 | 1.5E+01 | 1.7E+01 | 1.2E+01 |
| 4.44E+01 | 3.6E-02 | 1.15E-01 | 8.60E-02 | 9.0E-01 | 4.8E-02 | 1.3E+01 | 1.5E+01 | 1.6E+01 | 1.4E+01 |
| 5.55E+01 | 4.3E-02 | 1.15E-01 | 1.25E-01 | 8.1E-01 | 6.2E-02 | 1.5E+01 | 1.5E+01 | 1.4E+01 | 1.5E+01 |
| 6.94E+01 | 4.9E-02 | 1.15E-01 | 1.70E-01 | 7.2E-01 | 7.8E-02 | 1.6E+01 | 1.5E+01 | 1.3E+01 | 1.5E+01 |
| 8.67E+01 | 5.3E-02 | 1.15E-01 | 2.19E-01 | 6.5E-01 | 9.2E-02 | 1.7E+01 | 1.5E+01 | 1.2E+01 | 1.6E+01 |
| 1.08E+02 | 5.5E-02 | 1.15E-01 | 2.72E-01 | 5.8E-01 | 1.0E-01 | 1.8E+01 | 1.5E+01 | 1.1E+01 | 1.6E+01 |
| 1.36E+02 | 5.6E-02 | 1.15E-01 | 3.26E-01 | 5.2E-01 | 1.2E-01 | 1.9E+01 | 1.5E+01 | 9.8E+00 | 1.5E+01 |
| 1.69E+02 | 5.5E-02 | 1.15E-01 | 3.79E-01 | 4.6E-01 | 1.2E-01 | 2.0E+01 | 1.5E+01 | 8.8E+00 | 1.5E+01 |
| 2.12E+02 | 5.3E-02 | 1.15E-01 | 4.32E-01 | 4.1E-01 | 1.3E-01 | 2.1E+01 | 1.5E+01 | 7.9E+00 | 1.4E+01 |
| 2.65E+02 | 5.0E-02 | 1.15E-01 | 4.82E-01 | 3.7E-01 | 1.3E-01 | 2.2E+01 | 1.5E+01 | 7.1E+00 | 1.3E+01 |
| 3.31E+02 | 4.7E-02 | 1.15E-01 | 5.29E-01 | 3.3E-01 | 1.3E-01 | 2.3E+01 | 1.5E+01 | 6.4E+00 | 1.2E+01 |
| 4.14E+02 | 4.4E-02 | 1.15E-01 | 5.74E-01 | 3.0E-01 | 1.3E-01 | 2.4E+01 | 1.5E+01 | 5.7E+00 | 1.0E+01 |
| 5.17E+02 | 4.1E-02 | 1.15E-01 | 6.15E-01 | 2.6E-01 | 1.3E-01 | 2.4E+01 | 1.5E+01 | 5.1E+00 | 9.3E+00 |
| 6.46E+02 | 3.7E-02 | 1.15E-01 | 6.53E-01 | 2.4E-01 | 1.2E-01 | 2.5E+01 | 1.5E+01 | 4.6E+00 | 8.3E+00 |
| 8.08E+02 | 3.4E-02 | 1.15E-01 | 6.87E-01 | 2.1E-01 | 1.2E-01 | 2.5E+01 | 1.5E+01 | 4.1E+00 | 7.3E+00 |
| 1.01E+03 | 3.1E-02 | 1.15E-01 | 7.19E-01 | 1.9E-01 | 1.1E-01 | 2.6E+01 | 1.5E+01 | 3.7E+00 | 6.4E+00 |
| 1.26E+03 | 2.8E-02 | 1.15E-01 | 7.47E-01 | 1.7E-01 | 1.1E-01 | 2.6E+01 | 1.5E+01 | 3.3E+00 | 5.6E+00 |
| 1.58E+03 | 2.5E-02 | 1.15E-01 | 7.73E-01 | 1.5E-01 | 1.0E-01 | 2.7E+01 | 1.5E+01 | 3.0E+00 | 4.9E+00 |
| 1.97E+03 | 2.3E-02 | 1.15E-01 | 7.97E-01 | 1.4E-01 | 9.4E-02 | 2.7E+01 | 1.5E+01 | 2.7E+00 | 4.3E+00 |
| 2.47E+03 | 2.1E-02 | 1.15E-01 | 8.18E-01 | 1.2E-01 | 8.8E-02 | 2.7E+01 | 1.5E+01 | 2.4E+00 | 3.7E+00 |
| 3.08E+03 | 1.9E-02 | 1.15E-01 | 8.37E-01 | 1.1E-01 | 8.1E-02 | 2.8E+01 | 1.5E+01 | 2.1E+00 | 3.2E+00 |
| 3.85E+03 | 1.7E-02 | 1.15E-01 | 8.54E-01 | 9.7E-02 | 7.5E-02 | 2.8E+01 | 1.5E+01 | 1.9E+00 | 2.8E+00 |
| 4.81E+03 | 1.5E-02 | 1.15E-01 | 8.69E-01 | 8.7E-02 | 6.9E-02 | 2.8E+01 | 1.5E+01 | 1.7E+00 | 2.5E+00 |
| 6.02E+03 | 1.3E-02 | 1.15E-01 | 8.83E-01 | 7.7E-02 | 6.3E-02 | 2.8E+01 | 1.5E+01 | 1.5E+00 | 2.1E+00 |
| 7.52E+03 | 1.2E-02 | 1.15E-01 | 8.95E-01 | 6.9E-02 | 5.8E-02 | 2.9E+01 | 1.5E+01 | 1.4E+00 | 1.9E+00 |
| 9.40E+03 | 1.1E-02 | 1.15E-01 | 9.06E-01 | 6.2E-02 | 5.3E-02 | 2.9E+01 | 1.5E+01 | 1.2E+00 | 1.6E+00 |
| 1.18E+04 | 9.6E-03 | 1.15E-01 | 9.16E-01 | 5.5E-02 | 4.8E-02 | 2.9E+01 | 1.5E+01 | 1.1E+00 | 1.4E+00 |
| 1.47E+04 | 8.6E-03 | 1.15E-01 | 9.25E-01 | 5.0E-02 | 4.3E-02 | 2.9E+01 | 1.5E+01 | 9.7E-01 | 1.3E+00 |
| 1.84E+04 | 7.7E-03 | 1.15E-01 | 9.33E-01 | 4.4E-02 | 3.9E-02 | 2.9E+01 | 1.5E+01 | 8.7E-01 | 1.1E+00 |
| 2.30E+04 | 6.9E-03 | 1.15E-01 | 9.40E-01 | 4.0E-02 | 3.6E-02 | 2.9E+01 | 1.5E+01 | 7.8E-01 | 9.7E-01 |
| 2.87E+04 | 6.2E-03 | 1.15E-01 | 9.46E-01 | 3.5E-02 | 3.2E-02 | 2.9E+01 | 1.5E+01 | 7.0E-01 | 8.5E-01 |
| 3.59E+04 | 5.5E-03 | 1.15E-01 | 9.52E-01 | 3.2E-02 | 2.9E-02 | 2.9E+01 | 1.5E+01 | 6.2E-01 | 7.5E-01 |
| 4.48E+04 | 5.0E-03 | 1.15E-01 | 9.57E-01 | 2.8E-02 | 2.6E-02 | 3.0E+01 | 1.5E+01 | 5.6E-01 | 6.6E-01 |
| 5.61E+04 | 4.4E-03 | 1.15E-01 | 9.61E-01 | 2.5E-02 | 2.4E-02 | 3.0E+01 | 1.5E+01 | 5.0E-01 | 5.8E-01 |
| 7.01E+04 | 4.0E-03 | 1.15E-01 | 9.66E-01 | 2.3E-02 | 2.1E-02 | 3.0E+01 | 1.5E+01 | 4.5E-01 | 5.2E-01 |
| 8.76E+04 | 3.6E-03 | 1.15E-01 | 9.69E-01 | 2.0E-02 | 1.9E-02 | 3.0E+01 | 1.5E+01 | 4.0E-01 | 4.6E-01 |
| 1.09E+05 | 3.2E-03 | 1.15E-01 | 9.72E-01 | 1.8E-02 | 1.7E-02 | 3.0E+01 | 1.5E+01 | 3.6E-01 | 4.0E-01 |
| 1.37E+05 | 2.8E-03 | 1.15E-01 | 9.75E-01 | 1.6E-02 | 1.6E-02 | 3.0E+01 | 1.5E+01 | 3.2E-01 | 3.6E-01 |
| 1.71E+05 | 2.5E-03 | 1.15E-01 | 9.78E-01 | 1.5E-02 | 1.4E-02 | 3.0E+01 | 1.5E+01 | 2.9E-01 | 3.2E-01 |
| 2.14E+05 | 2.3E-03 | 1.15E-01 | 9.80E-01 | 1.3E-02 | 1.3E-02 | 3.0E+01 | 1.5E+01 | 2.6E-01 | 2.8E-01 |
| 2.67E+05 | 2.0E-03 | 1.15E-01 | 9.82E-01 | 1.2E-02 | 1.1E-02 | 3.0E+01 | 1.5E+01 | 2.3E-01 | 2.5E-01 |
| 3.34E+05 | 1.8E-03 | 1.15E-01 | 9.84E-01 | 1.0E-02 | 1.0E-02 | 3.0E+01 | 1.5E+01 | 2.0E-01 | 2.2E-01 |
| 4.18E+05 | 1.6E-03 | 1.15E-01 | 9.86E-01 | 9.3E-03 | 9.1E-03 | 3.0E+01 | 1.5E+01 | 1.8E-01 | 2.0E-01 |
| 5.22E+05 | 1.5E-03 | 1.15E-01 | 9.87E-01 | 8.3E-03 | 8.1E-03 | 3.0E+01 | 1.5E+01 | 1.6E-01 | 1.7E-01 |
| 6.53E+05 | 1.3E-03 | 1.15E-01 | 9.89E-01 | 7.4E-03 | 7.3E-03 | 3.0E+01 | 1.5E+01 | 1.5E-01 | 1.6E-01 |
| 8.16E+05 | 1.2E-03 | 1.15E-01 | 9.90E-01 | 6.7E-03 | 6.5E-03 | 3.0E+01 | 1.5E+01 | 1.3E-01 | 1.4E-01 |
| 1.02E+06 | 1.0E-03 | 1.15E-01 | 9.91E-01 | 6.0E-03 | 5.9E-03 | 3.0E+01 | 1.5E+01 | 1.2E-01 | 1.2E-01 |

# Appendix B - Parameters and calculations underlying Figure 6b

| | | |
|---|---|---|
| **Saltstone grout** | | |
| initial concentration, c | 1 | mol/L |
| porosity, n | 0.6 | unitless |
| effective diffusion coefficient, D | 1.0E-07 | $cm^2/s$ |
| $n\sqrt{D}$ | 1.90E-04 | $cm/\sqrt{s}$ |
| distribution coefficient, Kd | **3** | mL/g |
| grain density, $\rho_s$ | 2.6 | g/mL |
| retardation factor, R | 6.2 | unitless |
| retarded diffusion coefficient, $D_R$ | 1.6E-08 | $cm^2/s$ |
| $n\sqrt{D_R}$ | 7.62E-05 | $cm/\sqrt{s}$ |
| **Vault concrete** | | |
| initial concentration, c | 0 | mol/L |
| porosity, n | 0.18 | unitless |
| effective diffusion coefficient, D | 5.0E-08 | $cm^2/s$ |
| $n\sqrt{D}$ | 4.02E-05 | $cm/\sqrt{s}$ |
| distribution coefficient, Kd | **3** | mL/g |
| grain density, $\rho_s$ | 2.6 | g/mL |
| retardation factor, R | 36.5 | unitless |
| retarded diffusion coefficient, $D_R$ | 1.4E-09 | $cm^2/s$ |
| $n\sqrt{D_R}$ | 6.66E-06 | $cm/\sqrt{s}$ |
| **Interface** | | |
| concentration, c | 0.920 | mol/L |
| **Decay** | | |
| half-life, τ | **1.00E+08** | yr |
| decay rate, λ | 6.93E-09 | $yr^{-1}$ |
| **Flux** | | |
| area, A | 1 | $m^2$ |
| | 10000 | $cm^2$ |
| thickness, x | 8 | in |
| | 20.3 | cm |
| time factor | 1.25 | |
| concentration, c | 0.920 | mol/L |
| | 0.00092 | $mol/cm^3$ |
| effective diffusion coefficient, D | 1.4E-09 | $cm^2/s$ |
| | 0.04 | $cm^2/yr$ |
| steady-state flux | 3.52E-03 | mol/yr |
| concentration, c | 1.000 | mol/L |
| | 0.001 | $mol/cm^3$ |
| effective diffusion coefficient, D | 1.6E-08 | $cm^2/s$ |
| | 0.51 | $cm^2/yr$ |

| time | Short Term flux | Intermediate flux | conc | Long Term flux | Blended flux | Short Term mass | Intermediate mass | Long Term mass | Blended mass |
|---|---|---|---|---|---|---|---|---|---|
| yr | mol/yr | mol/yr | | mol/yr | mol/yr | mol | mol | mol | mol |
| 0.00E+00 | | | | | | | | | |
| 1.00E+00 | 0.0E+00 | 1.28E-01 | #NUM! | 1.5E+01 | #NUM! | #NUM! | 6.1E+02 | 1.3E+03 | #NUM! |
| 1.25E+00 | 0.0E+00 | 1.28E-01 | #NUM! | 1.3E+01 | #NUM! | #NUM! | 6.1E+02 | 1.3E+03 | #NUM! |
| 1.56E+00 | 0.0E+00 | 1.28E-01 | #NUM! | 1.2E+01 | #NUM! | #NUM! | 6.1E+02 | 1.3E+03 | #NUM! |
| 1.95E+00 | 0.0E+00 | 1.28E-01 | #NUM! | 1.1E+01 | #NUM! | #NUM! | 6.1E+02 | 1.3E+03 | #NUM! |
| 2.44E+00 | 0.0E+00 | 1.28E-01 | #NUM! | 9.6E+00 | #NUM! | #NUM! | 6.1E+02 | 1.3E+03 | #NUM! |
| 3.05E+00 | 0.0E+00 | 1.28E-01 | #NUM! | 8.6E+00 | #NUM! | #NUM! | 6.1E+02 | 1.2E+03 | #NUM! |
| 3.81E+00 | 1.9E-272 | 1.28E-01 | 0.00E+00 | 7.7E+00 | 1.9E-272 | 2.8E+01 | 6.1E+02 | 1.2E+03 | 2.8E+01 |
| 4.77E+00 | 4.8E-218 | 1.28E-01 | 0.00E+00 | 6.9E+00 | 4.8E-218 | 3.1E+01 | 6.1E+02 | 1.2E+03 | 3.1E+01 |
| 5.96E+00 | 1.6E-174 | 1.28E-01 | 0.00E+00 | 6.1E+00 | 1.6E-174 | 3.5E+01 | 6.1E+02 | 1.2E+03 | 3.5E+01 |
| 7.45E+00 | 1.0E-139 | 1.28E-01 | 0.00E+00 | 5.5E+00 | 1.0E-139 | 3.9E+01 | 6.1E+02 | 1.2E+03 | 3.9E+01 |
| 9.31E+00 | 6.9E-112 | 1.28E-01 | 0.00E+00 | 4.9E+00 | 6.9E-112 | 4.3E+01 | 6.1E+02 | 1.2E+03 | 4.3E+01 |
| 1.16E+01 | 1.2E-89 | 1.28E-01 | 0.00E+00 | 4.4E+00 | 1.2E-89 | 4.8E+01 | 6.1E+02 | 1.2E+03 | 4.8E+01 |
| 1.46E+01 | 7.8E-72 | 1.28E-01 | 0.00E+00 | 3.9E+00 | 7.8E-72 | 5.4E+01 | 6.1E+02 | 1.1E+03 | 5.4E+01 |
| 1.82E+01 | 1.3E-57 | 1.28E-01 | 0.00E+00 | 3.5E+00 | 1.3E-57 | 6.0E+01 | 6.1E+02 | 1.1E+03 | 6.0E+01 |
| 2.27E+01 | 3.1E-46 | 1.28E-01 | 0.00E+00 | 3.1E+00 | 3.1E-46 | 6.8E+01 | 6.1E+02 | 1.1E+03 | 6.8E+01 |
| 2.84E+01 | 3.8E-37 | 1.28E-01 | 0.00E+00 | 2.8E+00 | 3.8E-37 | 7.6E+01 | 6.1E+02 | 1.1E+03 | 7.6E+01 |
| 3.55E+01 | 6.9E-30 | 1.28E-01 | 0.00E+00 | 2.5E+00 | 6.9E-30 | 8.4E+01 | 6.1E+02 | 1.0E+03 | 8.4E+01 |
| 4.44E+01 | 4.3E-24 | 1.28E-01 | 0.00E+00 | 2.2E+00 | 4.3E-24 | 9.4E+01 | 6.1E+02 | 9.8E+02 | 9.4E+01 |
| 5.55E+01 | 1.8E-19 | 1.28E-01 | 0.00E+00 | 2.0E+00 | 1.8E-19 | 1.1E+02 | 6.1E+02 | 9.4E+02 | 1.1E+02 |
| 6.94E+01 | 9.1E-16 | 1.28E-01 | 1.11E-16 | 1.8E+00 | 9.1E-16 | 1.2E+02 | 6.1E+02 | 9.0E+02 | 1.2E+02 |
| 8.67E+01 | 8.1E-13 | 1.28E-01 | 1.12E-13 | 1.6E+00 | 8.1E-13 | 1.3E+02 | 6.1E+02 | 8.5E+02 | 1.3E+02 |
| 1.08E+02 | 1.8E-10 | 1.28E-01 | 3.09E-11 | 1.4E+00 | 1.8E-10 | 1.5E+02 | 6.1E+02 | 8.0E+02 | 1.5E+02 |
| 1.36E+02 | 1.3E-08 | 1.28E-01 | 2.83E-09 | 1.3E+00 | 1.3E-08 | 1.7E+02 | 6.1E+02 | 7.5E+02 | 1.7E+02 |
| 1.69E+02 | 4.0E-07 | 1.28E-01 | 1.07E-07 | 1.2E+00 | 4.0E-07 | 1.8E+02 | 6.1E+02 | 6.9E+02 | 1.8E+02 |
| 2.12E+02 | 6.1E-06 | 1.28E-01 | 2.01E-06 | 1.0E+00 | 6.1E-06 | 2.1E+02 | 6.1E+02 | 6.4E+02 | 2.1E+02 |
| 2.65E+02 | 5.2E-05 | 1.28E-01 | 2.13E-05 | 9.2E-01 | 5.2E-05 | 2.3E+02 | 6.1E+02 | 5.9E+02 | 2.3E+02 |
| 3.31E+02 | 2.8E-04 | 1.28E-01 | 1.43E-04 | 8.2E-01 | 2.8E-04 | 2.6E+02 | 6.1E+02 | 5.4E+02 | 2.6E+02 |
| 4.14E+02 | 1.1E-03 | 1.28E-01 | 6.72E-04 | 7.4E-01 | 1.1E-03 | 2.9E+02 | 6.1E+02 | 4.9E+02 | 2.9E+02 |
| 5.17E+02 | 3.1E-03 | 1.28E-01 | 2.35E-03 | 6.6E-01 | 3.1E-03 | 3.2E+02 | 6.1E+02 | 4.4E+02 | 3.2E+02 |
| 6.46E+02 | 6.9E-03 | 1.28E-01 | 6.52E-03 | 5.9E-01 | 7.1E-03 | 3.6E+02 | 6.1E+02 | 4.0E+02 | 3.6E+02 |
| 8.08E+02 | 1.3E-02 | 1.28E-01 | 1.50E-02 | 5.3E-01 | 1.4E-02 | 4.0E+02 | 6.1E+02 | 3.6E+02 | 4.0E+02 |
| 1.01E+03 | 2.1E-02 | 1.28E-01 | 2.95E-02 | 4.7E-01 | 2.3E-02 | 4.4E+02 | 6.1E+02 | 3.3E+02 | 4.4E+02 |
| 1.26E+03 | 3.0E-02 | 1.28E-01 | 5.16E-02 | 4.2E-01 | 3.4E-02 | 4.9E+02 | 6.1E+02 | 2.9E+02 | 4.8E+02 |
| 1.58E+03 | 3.9E-02 | 1.28E-01 | 8.16E-02 | 3.8E-01 | 4.7E-02 | 5.4E+02 | 6.1E+02 | 2.6E+02 | 5.1E+02 |
| 1.97E+03 | 4.7E-02 | 1.28E-01 | 1.19E-01 | 3.4E-01 | 6.0E-02 | 5.9E+02 | 6.1E+02 | 2.4E+02 | 5.3E+02 |
| 2.47E+03 | 5.4E-02 | 1.28E-01 | 1.64E-01 | 3.0E-01 | 7.2E-02 | 6.4E+02 | 6.1E+02 | 2.1E+02 | 5.3E+02 |
| 3.08E+03 | 5.9E-02 | 1.28E-01 | 2.13E-01 | 2.7E-01 | 8.1E-02 | 6.9E+02 | 6.1E+02 | 1.9E+02 | 5.2E+02 |
| 3.85E+03 | 6.1E-02 | 1.28E-01 | 2.65E-01 | 2.4E-01 | 8.8E-02 | 7.3E+02 | 6.1E+02 | 1.7E+02 | 5.0E+02 |
| 4.81E+03 | 6.2E-02 | 1.28E-01 | 3.19E-01 | 2.2E-01 | 9.2E-02 | 7.8E+02 | 6.1E+02 | 1.5E+02 | 4.6E+02 |
| 6.02E+03 | 6.1E-02 | 1.28E-01 | 3.73E-01 | 1.9E-01 | 9.4E-02 | 8.2E+02 | 6.1E+02 | 1.4E+02 | 4.2E+02 |
| 7.52E+03 | 5.9E-02 | 1.28E-01 | 4.25E-01 | 1.7E-01 | 9.4E-02 | 8.6E+02 | 6.1E+02 | 1.2E+02 | 3.8E+02 |
| 9.40E+03 | 5.7E-02 | 1.28E-01 | 4.76E-01 | 1.5E-01 | 9.1E-02 | 8.9E+02 | 6.1E+02 | 1.1E+02 | 3.3E+02 |
| 1.18E+04 | 5.3E-02 | 1.28E-01 | 5.24E-01 | 1.4E-01 | 8.8E-02 | 9.3E+02 | 6.1E+02 | 9.9E+01 | 2.9E+02 |
| 1.47E+04 | 5.0E-02 | 1.28E-01 | 5.68E-01 | 1.2E-01 | 8.3E-02 | 9.6E+02 | 6.1E+02 | 8.8E+01 | 2.5E+02 |
| 1.84E+04 | 4.6E-02 | 1.28E-01 | 6.10E-01 | 1.1E-01 | 7.8E-02 | 9.8E+02 | 6.1E+02 | 7.9E+01 | 2.1E+02 |
| 2.30E+04 | 4.2E-02 | 1.28E-01 | 6.48E-01 | 9.9E-02 | 7.3E-02 | 1.0E+03 | 6.1E+02 | 7.1E+01 | 1.8E+02 |
| 2.87E+04 | 3.8E-02 | 1.28E-01 | 6.83E-01 | 8.8E-02 | 6.8E-02 | 1.0E+03 | 6.1E+02 | 6.3E+01 | 1.5E+02 |
| 3.59E+04 | 3.5E-02 | 1.28E-01 | 7.15E-01 | 7.9E-02 | 6.3E-02 | 1.1E+03 | 6.1E+02 | 5.7E+01 | 1.3E+02 |
| 4.48E+04 | 3.2E-02 | 1.28E-01 | 7.44E-01 | 7.1E-02 | 5.8E-02 | 1.1E+03 | 6.1E+02 | 5.1E+01 | 1.1E+02 |
| 5.61E+04 | 2.9E-02 | 1.28E-01 | 7.70E-01 | 6.3E-02 | 5.3E-02 | 1.1E+03 | 6.1E+02 | 4.5E+01 | 9.4E+01 |
| 7.01E+04 | 2.6E-02 | 1.28E-01 | 7.94E-01 | 5.7E-02 | 4.8E-02 | 1.1E+03 | 6.1E+02 | 4.1E+01 | 8.0E+01 |
| 8.76E+04 | 2.3E-02 | 1.28E-01 | 8.15E-01 | 5.1E-02 | 4.4E-02 | 1.1E+03 | 6.1E+02 | 3.6E+01 | 6.8E+01 |
| 1.09E+05 | 2.1E-02 | 1.28E-01 | 8.34E-01 | 4.5E-02 | 4.0E-02 | 1.1E+03 | 6.1E+02 | 3.2E+01 | 5.8E+01 |
| 1.37E+05 | 1.9E-02 | 1.28E-01 | 8.52E-01 | 4.0E-02 | 3.6E-02 | 1.1E+03 | 6.1E+02 | 2.9E+01 | 5.0E+01 |
| 1.71E+05 | 1.7E-02 | 1.28E-01 | 8.67E-01 | 3.6E-02 | 3.3E-02 | 1.1E+03 | 6.1E+02 | 2.6E+01 | 4.3E+01 |
| 2.14E+05 | 1.5E-02 | 1.28E-01 | 8.81E-01 | 3.2E-02 | 3.0E-02 | 1.2E+03 | 6.1E+02 | 2.3E+01 | 3.7E+01 |
| 2.67E+05 | 1.4E-02 | 1.28E-01 | 8.94E-01 | 2.9E-02 | 2.7E-02 | 1.2E+03 | 6.1E+02 | 2.1E+01 | 3.2E+01 |
| 3.34E+05 | 1.2E-02 | 1.28E-01 | 9.05E-01 | 2.6E-02 | 2.4E-02 | 1.2E+03 | 6.1E+02 | 1.9E+01 | 2.8E+01 |
| 4.18E+05 | 1.1E-02 | 1.28E-01 | 9.15E-01 | 2.3E-02 | 2.2E-02 | 1.2E+03 | 6.1E+02 | 1.7E+01 | 2.4E+01 |
| 5.22E+05 | 9.7E-03 | 1.28E-01 | 9.24E-01 | 2.1E-02 | 1.9E-02 | 1.2E+03 | 6.1E+02 | 1.5E+01 | 2.1E+01 |
| 6.53E+05 | 8.7E-03 | 1.28E-01 | 9.32E-01 | 1.8E-02 | 1.8E-02 | 1.2E+03 | 6.1E+02 | 1.3E+01 | 1.8E+01 |
| 8.16E+05 | 7.8E-03 | 1.28E-01 | 9.39E-01 | 1.6E-02 | 1.6E-02 | 1.2E+03 | 6.1E+02 | 1.2E+01 | 1.6E+01 |
| 1.02E+06 | 7.0E-03 | 1.28E-01 | 9.45E-01 | 1.5E-02 | 1.4E-02 | 1.2E+03 | 6.1E+02 | 1.1E+01 | 1.4E+01 |

# Appendix C - Parameters and calculations underlying Figure 6c

| | | |
|---|---|---|
| **Saltstone grout** | | |
| initial concentration, c | 1 | mol/L |
| porosity, n | 0.6 | unitless |
| effective diffusion coefficient, D | 1.0E-07 | $cm^2/s$ |
| $n\sqrt{D}$ | 1.90E-04 | $cm/\sqrt{s}$ |
| distribution coefficient, Kd | **0** | mL/g |
| grain density, $\rho_s$ | 2.6 | g/mL |
| retardation factor, R | 1.0 | unitless |
| retarded diffusion coefficient, $D_R$ | 1.0E-07 | $cm^2/s$ |
| $n\sqrt{D_R}$ | 1.90E-04 | $cm/\sqrt{s}$ |
| **Vault concrete** | | |
| initial concentration, c | 0 | mol/L |
| porosity, n | 0.18 | unitless |
| effective diffusion coefficient, D | 5.0E-08 | $cm^2/s$ |
| $n\sqrt{D}$ | 4.02E-05 | $cm/\sqrt{s}$ |
| distribution coefficient, Kd | **0** | mL/g |
| grain density, $\rho_s$ | 2.6 | g/mL |
| retardation factor, R | 1.0 | unitless |
| retarded diffusion coefficient, $D_R$ | 5.0E-08 | $cm^2/s$ |
| $n\sqrt{D_R}$ | 4.02E-05 | $cm/\sqrt{s}$ |
| **Interface** | | |
| concentration, c | 0.825 | mol/L |
| **Decay** | | |
| half-life, $\tau$ | **1.00E+03** | yr |
| decay rate, $\lambda$ | 0.000693 | $yr^{-1}$ |
| **Flux** | | |
| area, A | 1 | $m^2$ |
| | 10000 | $cm^2$ |
| thickness, x | 8 | in |
| | 20.3 | cm |
| time factor | 1.25 | |
| concentration, c | 0.825 | mol/L |
| | 0.000825 | $mol/cm^3$ |
| effective diffusion coefficient, D | 5.0E-08 | $cm^2/s$ |
| | 1.58 | $cm^2/yr$ |
| steady-state flux | 1.15E-01 | mol/yr |
| concentration, c | 1.000 | mol/L |
| | 0.001 | $mol/cm^3$ |
| effective diffusion coefficient, D | 1.0E-07 | $cm^2/s$ |
| | 3.15 | $cm^2/yr$ |

| time | Short Term flux | Intermediate flux | conc | Long Term flux | Blended flux | Short Term mass | Intermediate mass | Long Term mass | Blended mass |
|---|---|---|---|---|---|---|---|---|---|
| yr | mol/yr | mol/yr | | mol/yr | mol/yr | mol | mol | mol | mol |
| 0.00E+00 | | | | | | | | | |
| 1.00E+00 | 3.9E-29 | 1.15E-01 | 0.00E+00 | 6.0E+00 | 3.9E-29 | 2.1E+00 | 1.5E+01 | 3.3E+01 | 2.1E+00 |
| 1.25E+00 | 1.7E-23 | 1.15E-01 | 0.00E+00 | 5.4E+00 | 1.7E-23 | 2.4E+00 | 1.5E+01 | 3.3E+01 | 2.4E+00 |
| 1.56E+00 | 5.4E-19 | 1.15E-01 | 0.00E+00 | 4.8E+00 | 5.4E-19 | 2.6E+00 | 1.5E+01 | 3.2E+01 | 2.6E+00 |
| 1.95E+00 | 2.1E-15 | 1.15E-01 | 2.22E-16 | 4.3E+00 | 2.1E-15 | 2.9E+00 | 1.5E+01 | 3.1E+01 | 2.9E+00 |
| 2.44E+00 | 1.5E-12 | 1.15E-01 | 2.42E-13 | 3.8E+00 | 1.5E-12 | 3.3E+00 | 1.5E+01 | 3.1E+01 | 3.3E+00 |
| 3.05E+00 | 2.9E-10 | 1.15E-01 | 5.75E-11 | 3.4E+00 | 2.9E-10 | 3.7E+00 | 1.5E+01 | 3.0E+01 | 3.7E+00 |
| 3.81E+00 | 1.9E-08 | 1.15E-01 | 4.67E-09 | 3.1E+00 | 1.9E-08 | 4.1E+00 | 1.5E+01 | 2.9E+01 | 4.1E+00 |
| 4.77E+00 | 5.2E-07 | 1.15E-01 | 1.61E-07 | 2.7E+00 | 5.2E-07 | 4.6E+00 | 1.5E+01 | 2.9E+01 | 4.6E+00 |
| 5.96E+00 | 7.3E-06 | 1.15E-01 | 2.77E-06 | 2.5E+00 | 7.3E-06 | 5.1E+00 | 1.5E+01 | 2.8E+01 | 5.1E+00 |
| 7.45E+00 | 5.9E-05 | 1.15E-01 | 2.76E-05 | 2.2E+00 | 5.9E-05 | 5.7E+00 | 1.5E+01 | 2.7E+01 | 5.7E+00 |
| 9.31E+00 | 3.0E-04 | 1.14E-01 | 1.77E-04 | 2.0E+00 | 3.0E-04 | 6.4E+00 | 1.5E+01 | 2.5E+01 | 6.4E+00 |
| 1.16E+01 | 1.1E-03 | 1.14E-01 | 7.98E-04 | 1.7E+00 | 1.1E-03 | 7.1E+00 | 1.5E+01 | 2.4E+01 | 7.1E+00 |
| 1.46E+01 | 3.0E-03 | 1.14E-01 | 2.70E-03 | 1.6E+00 | 3.1E-03 | 7.9E+00 | 1.5E+01 | 2.3E+01 | 8.0E+00 |
| 1.82E+01 | 6.7E-03 | 1.14E-01 | 7.30E-03 | 1.4E+00 | 6.9E-03 | 8.8E+00 | 1.5E+01 | 2.1E+01 | 8.9E+00 |
| 2.27E+01 | 1.2E-02 | 1.13E-01 | 1.64E-02 | 1.2E+00 | 1.3E-02 | 9.8E+00 | 1.5E+01 | 2.0E+01 | 9.9E+00 |
| 2.84E+01 | 1.9E-02 | 1.13E-01 | 3.18E-02 | 1.1E+00 | 2.2E-02 | 1.1E+01 | 1.5E+01 | 1.8E+01 | 1.1E+01 |
| 3.55E+01 | 2.7E-02 | 1.12E-01 | 5.49E-02 | 9.8E-01 | 3.3E-02 | 1.2E+01 | 1.5E+01 | 1.7E+01 | 1.2E+01 |
| 4.44E+01 | 3.5E-02 | 1.12E-01 | 8.60E-02 | 8.7E-01 | 4.6E-02 | 1.3E+01 | 1.5E+01 | 1.5E+01 | 1.3E+01 |
| 5.55E+01 | 4.2E-02 | 1.11E-01 | 1.25E-01 | 7.8E-01 | 6.0E-02 | 1.4E+01 | 1.5E+01 | 1.4E+01 | 1.4E+01 |
| 6.94E+01 | 4.7E-02 | 1.10E-01 | 1.70E-01 | 6.9E-01 | 7.4E-02 | 1.5E+01 | 1.4E+01 | 1.3E+01 | 1.5E+01 |
| 8.67E+01 | 5.0E-02 | 1.09E-01 | 2.19E-01 | 6.1E-01 | 8.6E-02 | 1.6E+01 | 1.4E+01 | 1.1E+01 | 1.5E+01 |
| 1.08E+02 | 5.1E-02 | 1.07E-01 | 2.72E-01 | 5.4E-01 | 9.7E-02 | 1.7E+01 | 1.4E+01 | 1.0E+01 | 1.5E+01 |
| 1.36E+02 | 5.1E-02 | 1.05E-01 | 3.26E-01 | 4.7E-01 | 1.0E-01 | 1.7E+01 | 1.4E+01 | 8.9E+00 | 1.4E+01 |
| 1.69E+02 | 4.9E-02 | 1.02E-01 | 3.79E-01 | 4.1E-01 | 1.1E-01 | 1.8E+01 | 1.3E+01 | 7.8E+00 | 1.3E+01 |
| 2.12E+02 | 4.6E-02 | 9.95E-02 | 4.32E-01 | 3.6E-01 | 1.1E-01 | 1.8E+01 | 1.3E+01 | 6.8E+00 | 1.2E+01 |
| 2.65E+02 | 4.2E-02 | 9.59E-02 | 4.82E-01 | 3.1E-01 | 1.1E-01 | 1.8E+01 | 1.3E+01 | 5.9E+00 | 1.1E+01 |
| 3.31E+02 | 3.8E-02 | 9.16E-02 | 5.29E-01 | 2.6E-01 | 1.1E-01 | 1.8E+01 | 1.2E+01 | 5.1E+00 | 9.3E+00 |
| 4.14E+02 | 3.3E-02 | 8.65E-02 | 5.74E-01 | 2.2E-01 | 9.9E-02 | 1.8E+01 | 1.1E+01 | 4.3E+00 | 7.9E+00 |
| 5.17E+02 | 2.8E-02 | 8.05E-02 | 6.15E-01 | 1.8E-01 | 9.0E-02 | 1.7E+01 | 1.1E+01 | 3.6E+00 | 6.5E+00 |
| 6.46E+02 | 2.4E-02 | 7.36E-02 | 6.53E-01 | 1.5E-01 | 8.0E-02 | 1.6E+01 | 9.6E+00 | 2.9E+00 | 5.3E+00 |
| 8.08E+02 | 1.9E-02 | 6.58E-02 | 6.87E-01 | 1.2E-01 | 6.8E-02 | 1.5E+01 | 8.6E+00 | 2.4E+00 | 4.2E+00 |
| 1.01E+03 | 1.5E-02 | 5.72E-02 | 7.19E-01 | 9.4E-02 | 5.7E-02 | 1.3E+01 | 7.5E+00 | 1.8E+00 | 3.2E+00 |
| 1.26E+03 | 1.2E-02 | 4.80E-02 | 7.47E-01 | 7.1E-02 | 4.5E-02 | 1.1E+01 | 6.3E+00 | 1.4E+00 | 2.3E+00 |
| 1.58E+03 | 8.5E-03 | 3.86E-02 | 7.73E-01 | 5.1E-02 | 3.4E-02 | 9.0E+00 | 5.1E+00 | 9.9E-01 | 1.6E+00 |
| 1.97E+03 | 5.8E-03 | 2.94E-02 | 7.97E-01 | 3.5E-02 | 2.4E-02 | 6.9E+00 | 3.8E+00 | 6.8E-01 | 1.1E+00 |
| 2.47E+03 | 3.7E-03 | 2.09E-02 | 8.18E-01 | 2.2E-02 | 1.6E-02 | 5.0E+00 | 2.7E+00 | 4.3E-01 | 6.7E-01 |
| 3.08E+03 | 2.2E-03 | 1.36E-02 | 8.37E-01 | 1.3E-02 | 9.6E-03 | 3.3E+00 | 1.8E+00 | 2.5E-01 | 3.8E-01 |
| 3.85E+03 | 1.2E-03 | 7.98E-03 | 8.54E-01 | 6.7E-03 | 5.2E-03 | 1.9E+00 | 1.0E+00 | 1.3E-01 | 1.9E-01 |
| 4.81E+03 | 5.3E-04 | 4.09E-03 | 8.69E-01 | 3.1E-03 | 2.4E-03 | 1.0E+00 | 5.4E-01 | 6.0E-02 | 8.7E-02 |
| 6.02E+03 | 2.1E-04 | 1.78E-03 | 8.83E-01 | 1.2E-03 | 9.7E-04 | 4.4E-01 | 2.3E-01 | 2.3E-02 | 3.3E-02 |
| 7.52E+03 | 6.5E-05 | 6.26E-04 | 8.95E-01 | 3.8E-04 | 3.1E-04 | 1.6E-01 | 8.2E-02 | 7.4E-03 | 1.0E-02 |
| 9.40E+03 | 1.6E-05 | 1.70E-04 | 9.06E-01 | 9.2E-05 | 7.8E-05 | 4.2E-02 | 2.2E-02 | 1.8E-03 | 2.4E-03 |
| 1.18E+04 | 2.8E-06 | 3.33E-05 | 9.16E-01 | 1.6E-05 | 1.4E-05 | 8.4E-03 | 4.4E-03 | 3.1E-04 | 4.1E-04 |
| 1.47E+04 | 3.3E-07 | 4.35E-06 | 9.25E-01 | 1.9E-06 | 1.6E-06 | 1.1E-03 | 5.7E-04 | 3.7E-05 | 4.7E-05 |
| 1.84E+04 | 2.3E-08 | 3.41E-07 | 9.33E-01 | 1.3E-07 | 1.2E-07 | 8.6E-05 | 4.5E-05 | 2.6E-06 | 3.3E-06 |
| 2.30E+04 | 8.5E-10 | 1.41E-08 | 9.40E-01 | 4.9E-09 | 4.4E-09 | 3.6E-06 | 1.9E-06 | 9.6E-08 | 1.2E-07 |
| 2.87E+04 | 1.4E-11 | 2.65E-10 | 9.46E-01 | 8.1E-11 | 7.4E-11 | 6.7E-08 | 3.5E-08 | 1.6E-09 | 2.0E-09 |
| 3.59E+04 | 8.8E-14 | 1.83E-12 | 9.52E-01 | 5.0E-13 | 4.6E-13 | 4.7E-10 | 2.4E-10 | 9.9E-12 | 1.2E-11 |
| 4.48E+04 | 1.6E-16 | 3.66E-15 | 9.57E-01 | 9.0E-16 | 8.4E-16 | 9.4E-13 | 4.8E-13 | 1.8E-14 | 2.1E-14 |
| 5.61E+04 | 5.9E-20 | 1.54E-18 | 9.61E-01 | 3.4E-19 | 3.2E-19 | 4.0E-16 | 2.0E-16 | 6.7E-18 | 7.8E-18 |
| 7.01E+04 | 3.2E-24 | 9.33E-23 | 9.66E-01 | 1.8E-23 | 1.7E-23 | 2.4E-20 | 1.2E-20 | 3.6E-22 | 4.2E-22 |
| 8.76E+04 | 1.5E-29 | 4.98E-28 | 9.69E-01 | 8.8E-29 | 8.3E-29 | 1.3E-25 | 6.5E-26 | 1.7E-27 | 2.0E-27 |
| 1.09E+05 | 3.5E-36 | 1.28E-34 | 9.72E-01 | 2.0E-35 | 1.9E-35 | 3.3E-32 | 1.7E-32 | 4.0E-34 | 4.5E-34 |
| 1.37E+05 | 1.8E-44 | 7.36E-43 | 9.75E-01 | 1.0E-43 | 9.9E-44 | 1.9E-40 | 9.6E-41 | 2.0E-42 | 2.3E-42 |
| 1.71E+05 | 8.2E-55 | 3.70E-53 | 9.78E-01 | 4.7E-54 | 4.5E-54 | 9.6E-51 | 4.8E-51 | 9.2E-53 | 1.0E-52 |
| 2.14E+05 | 9.8E-68 | 4.95E-66 | 9.80E-01 | 5.6E-67 | 5.4E-67 | 1.3E-63 | 6.5E-64 | 1.1E-65 | 1.2E-65 |
| 2.67E+05 | 7.1E-84 | 4.01E-82 | 9.82E-01 | 4.0E-83 | 3.9E-83 | 1.0E-79 | 5.3E-80 | 8.0E-82 | 8.7E-82 |
| 3.34E+05 | 4.9E-104 | 3.08E-102 | 9.84E-01 | 2.8E-103 | 2.7E-103 | 8.0E-100 | 4.0E-100 | 5.5E-102 | 5.9E-102 |
| 4.18E+05 | 3.1E-129 | 2.22E-127 | 9.86E-01 | 1.8E-128 | 1.7E-128 | 5.8E-125 | 2.9E-125 | 3.5E-127 | 3.8E-127 |
| 5.22E+05 | 1.0E-160 | 8.25E-159 | 9.87E-01 | 6.0E-160 | 5.8E-160 | 2.1E-156 | 1.1E-156 | 1.2E-158 | 1.2E-158 |
| 6.53E+05 | 4.8E-200 | 4.27E-198 | 9.89E-01 | 2.8E-199 | 2.7E-199 | 1.1E-195 | 5.6E-196 | 5.4E-198 | 5.8E-198 |
| 8.16E+05 | 3.4E-249 | 3.33E-247 | 9.90E-01 | 1.9E-248 | 1.9E-248 | 8.7E-245 | 4.4E-245 | 3.8E-247 | 4.0E-247 |
| 1.02E+06 | 0.0E+00 | 0.00E+00 | 9.91E-01 | 0.0E+00 | #NUM! | 3.6E-306 | 1.8E-306 | 0.0E+00 | #NUM! |

# Appendix D - Parameters and calculations underlying Figure 6d

| | | |
|---|---|---|
| **Saltstone grout** | | |
| initial concentration, c | 1 | mol/L |
| porosity, n | 0.6 | unitless |
| effective diffusion coefficient, D | 1.0E-07 | $cm^2/s$ |
| $n\sqrt{D}$ | 1.90E-04 | $cm/\sqrt{s}$ |
| distribution coefficient, Kd | **3** | mL/g |
| grain density, $\rho_s$ | 2.6 | g/mL |
| retardation factor, R | 6.2 | unitless |
| retarded diffusion coefficient, $D_R$ | 1.6E-08 | $cm^2/s$ |
| $n\sqrt{D_R}$ | 7.62E-05 | $cm/\sqrt{s}$ |
| **Vault concrete** | | |
| initial concentration, c | 0 | mol/L |
| porosity, n | 0.18 | unitless |
| effective diffusion coefficient, D | 5.0E-08 | $cm^2/s$ |
| $n\sqrt{D}$ | 4.02E-05 | $cm/\sqrt{s}$ |
| distribution coefficient, Kd | **3** | mL/g |
| grain density, $\rho_s$ | 2.6 | g/mL |
| retardation factor, R | 36.5 | unitless |
| retarded diffusion coefficient, $D_R$ | 1.4E-09 | $cm^2/s$ |
| $n\sqrt{D_R}$ | 6.66E-06 | $cm/\sqrt{s}$ |
| **Interface** | | |
| concentration, c | 0.920 | mol/L |
| **Decay** | | |
| half-life, τ | **1.00E+03** | yr |
| decay rate, λ | 0.000693 | $yr^{-1}$ |
| **Flux** | | |
| area, A | 1 | $m^2$ |
| | 10000 | $cm^2$ |
| thickness, x | 8 | in |
| | 20.3 | cm |
| time factor | 1.25 | |
| concentration, c | 0.920 | mol/L |
| | 0.00092 | $mol/cm^3$ |
| effective diffusion coefficient, D | 1.4E-09 | $cm^2/s$ |
| | 0.04 | $cm^2/yr$ |
| steady-state flux | 3.52E-03 | mol/yr |
| concentration, c | 1.000 | mol/L |
| | 0.001 | $mol/cm^3$ |
| effective diffusion coefficient, D | 1.6E-08 | $cm^2/s$ |
| | 0.51 | $cm^2/yr$ |

| time | Short Term flux | Intermediate flux | conc | Long Term flux | Blended flux | Short Term mass | Intermediate mass | Long Term mass | Blended mass |
|---|---|---|---|---|---|---|---|---|---|
| yr | mol/yr | mol/yr | | mol/yr | mol/yr | mol | mol | mol | mol |
| 0.00E+00 | | | | | | | | | |
| 1.00E+00 | 0.0E+00 | 1.28E-01 | #NUM! | 1.5E+01 | #NUM! | #NUM! | 6.1E+02 | 1.3E+03 | #NUM! |
| 1.25E+00 | 0.0E+00 | 1.28E-01 | #NUM! | 1.3E+01 | #NUM! | #NUM! | 6.1E+02 | 1.3E+03 | #NUM! |
| 1.56E+00 | 0.0E+00 | 1.28E-01 | #NUM! | 1.2E+01 | #NUM! | #NUM! | 6.1E+02 | 1.3E+03 | #NUM! |
| 1.95E+00 | 0.0E+00 | 1.28E-01 | #NUM! | 1.1E+01 | #NUM! | #NUM! | 6.1E+02 | 1.3E+03 | #NUM! |
| 2.44E+00 | 0.0E+00 | 1.28E-01 | #NUM! | 9.6E+00 | #NUM! | #NUM! | 6.1E+02 | 1.3E+03 | #NUM! |
| 3.05E+00 | 0.0E+00 | 1.28E-01 | #NUM! | 8.6E+00 | #NUM! | #NUM! | 6.1E+02 | 1.2E+03 | #NUM! |
| 3.81E+00 | 1.9E-272 | 1.28E-01 | 0.00E+00 | 7.6E+00 | 1.9E-272 | 2.8E+01 | 6.1E+02 | 1.2E+03 | 2.8E+01 |
| 4.77E+00 | 4.8E-218 | 1.28E-01 | 0.00E+00 | 6.8E+00 | 4.8E-218 | 3.1E+01 | 6.1E+02 | 1.2E+03 | 3.1E+01 |
| 5.96E+00 | 1.6E-174 | 1.28E-01 | 0.00E+00 | 6.1E+00 | 1.6E-174 | 3.4E+01 | 6.1E+02 | 1.2E+03 | 3.4E+01 |
| 7.45E+00 | 1.0E-139 | 1.28E-01 | 0.00E+00 | 5.5E+00 | 1.0E-139 | 3.8E+01 | 6.1E+02 | 1.2E+03 | 3.8E+01 |
| 9.31E+00 | 6.8E-112 | 1.28E-01 | 0.00E+00 | 4.9E+00 | 6.8E-112 | 4.3E+01 | 6.1E+02 | 1.2E+03 | 4.3E+01 |
| 1.16E+01 | 1.2E-89 | 1.27E-01 | 0.00E+00 | 4.4E+00 | 1.2E-89 | 4.8E+01 | 6.1E+02 | 1.1E+03 | 4.8E+01 |
| 1.46E+01 | 7.7E-72 | 1.27E-01 | 0.00E+00 | 3.9E+00 | 7.7E-72 | 5.4E+01 | 6.1E+02 | 1.1E+03 | 5.4E+01 |
| 1.82E+01 | 1.3E-57 | 1.27E-01 | 0.00E+00 | 3.5E+00 | 1.3E-57 | 6.0E+01 | 6.1E+02 | 1.1E+03 | 6.0E+01 |
| 2.27E+01 | 3.0E-46 | 1.26E-01 | 0.00E+00 | 3.1E+00 | 3.0E-46 | 6.7E+01 | 6.0E+02 | 1.1E+03 | 6.7E+01 |
| 2.84E+01 | 3.7E-37 | 1.26E-01 | 0.00E+00 | 2.8E+00 | 3.7E-37 | 7.4E+01 | 6.0E+02 | 1.0E+03 | 7.4E+01 |
| 3.55E+01 | 6.7E-30 | 1.25E-01 | 0.00E+00 | 2.5E+00 | 6.7E-30 | 8.2E+01 | 6.0E+02 | 1.0E+03 | 8.2E+01 |
| 4.44E+01 | 4.2E-24 | 1.25E-01 | 0.00E+00 | 2.2E+00 | 4.2E-24 | 9.2E+01 | 6.0E+02 | 9.5E+02 | 9.2E+01 |
| 5.55E+01 | 1.8E-19 | 1.24E-01 | 0.00E+00 | 1.9E+00 | 1.8E-19 | 1.0E+02 | 5.9E+02 | 9.1E+02 | 1.0E+02 |
| 6.94E+01 | 8.7E-16 | 1.22E-01 | 1.11E-16 | 1.7E+00 | 8.7E-16 | 1.1E+02 | 5.9E+02 | 8.6E+02 | 1.1E+02 |
| 8.67E+01 | 7.6E-13 | 1.21E-01 | 1.12E-13 | 1.5E+00 | 7.6E-13 | 1.2E+02 | 5.8E+02 | 8.0E+02 | 1.2E+02 |
| 1.08E+02 | 1.7E-10 | 1.19E-01 | 3.09E-11 | 1.3E+00 | 1.7E-10 | 1.4E+02 | 5.7E+02 | 7.4E+02 | 1.4E+02 |
| 1.36E+02 | 1.2E-08 | 1.17E-01 | 2.83E-09 | 1.2E+00 | 1.2E-08 | 1.5E+02 | 5.6E+02 | 6.8E+02 | 1.5E+02 |
| 1.69E+02 | 3.6E-07 | 1.14E-01 | 1.07E-07 | 1.0E+00 | 3.6E-07 | 1.6E+02 | 5.5E+02 | 6.2E+02 | 1.6E+02 |
| 2.12E+02 | 5.2E-06 | 1.11E-01 | 2.01E-06 | 8.9E-01 | 5.2E-06 | 1.8E+02 | 5.3E+02 | 5.5E+02 | 1.8E+02 |
| 2.65E+02 | 4.3E-05 | 1.07E-01 | 2.13E-05 | 7.7E-01 | 4.3E-05 | 1.9E+02 | 5.1E+02 | 4.9E+02 | 1.9E+02 |
| 3.31E+02 | 2.2E-04 | 1.02E-01 | 1.43E-04 | 6.5E-01 | 2.3E-04 | 2.1E+02 | 4.9E+02 | 4.3E+02 | 2.1E+02 |
| 4.14E+02 | 8.1E-04 | 9.64E-02 | 6.72E-04 | 5.5E-01 | 8.1E-04 | 2.2E+02 | 4.6E+02 | 3.7E+02 | 2.2E+02 |
| 5.17E+02 | 2.1E-03 | 8.98E-02 | 2.35E-03 | 4.6E-01 | 2.2E-03 | 2.3E+02 | 4.3E+02 | 3.1E+02 | 2.3E+02 |
| 6.46E+02 | 4.4E-03 | 8.21E-02 | 6.52E-03 | 3.8E-01 | 4.5E-03 | 2.3E+02 | 3.9E+02 | 2.6E+02 | 2.3E+02 |
| 8.08E+02 | 7.4E-03 | 7.34E-02 | 1.50E-02 | 3.0E-01 | 7.8E-03 | 2.3E+02 | 3.5E+02 | 2.1E+02 | 2.3E+02 |
| 1.01E+03 | 1.0E-02 | 6.38E-02 | 2.95E-02 | 2.3E-01 | 1.1E-02 | 2.2E+02 | 3.1E+02 | 1.6E+02 | 2.2E+02 |
| 1.26E+03 | 1.3E-02 | 5.36E-02 | 5.16E-02 | 1.8E-01 | 1.4E-02 | 2.0E+02 | 2.6E+02 | 1.2E+02 | 2.0E+02 |
| 1.58E+03 | 1.3E-02 | 4.30E-02 | 8.16E-02 | 1.3E-01 | 1.6E-02 | 1.8E+02 | 2.1E+02 | 8.9E+01 | 1.7E+02 |
| 1.97E+03 | 1.2E-02 | 3.27E-02 | 1.19E-01 | 8.6E-02 | 1.5E-02 | 1.5E+02 | 1.6E+02 | 6.1E+01 | 1.3E+02 |
| 2.47E+03 | 9.8E-03 | 2.33E-02 | 1.64E-01 | 5.5E-02 | 1.3E-02 | 1.2E+02 | 1.1E+02 | 3.9E+01 | 9.7E+01 |
| 3.08E+03 | 6.9E-03 | 1.52E-02 | 2.13E-01 | 3.2E-02 | 9.6E-03 | 8.1E+01 | 7.3E+01 | 2.3E+01 | 6.2E+01 |
| 3.85E+03 | 4.3E-03 | 8.90E-03 | 2.65E-01 | 1.7E-02 | 6.1E-03 | 5.1E+01 | 4.3E+01 | 1.2E+01 | 3.5E+01 |
| 4.81E+03 | 2.2E-03 | 4.56E-03 | 3.19E-01 | 7.7E-03 | 3.3E-03 | 2.8E+01 | 2.2E+01 | 5.5E+00 | 1.6E+01 |
| 6.02E+03 | 9.5E-04 | 1.98E-03 | 3.73E-01 | 3.0E-03 | 1.5E-03 | 1.3E+01 | 9.5E+00 | 2.1E+00 | 6.5E+00 |
| 7.52E+03 | 3.2E-04 | 6.98E-04 | 4.25E-01 | 9.4E-04 | 5.1E-04 | 4.7E+00 | 3.3E+00 | 6.7E-01 | 2.0E+00 |
| 9.40E+03 | 8.4E-05 | 1.90E-04 | 4.76E-01 | 2.3E-04 | 1.3E-04 | 1.3E+00 | 9.1E-01 | 1.6E-01 | 4.9E-01 |
| 1.18E+04 | 1.5E-05 | 3.72E-05 | 5.24E-01 | 4.0E-05 | 2.5E-05 | 2.7E-01 | 1.8E-01 | 2.9E-02 | 8.3E-02 |
| 1.47E+04 | 1.9E-06 | 4.85E-06 | 5.68E-01 | 4.7E-06 | 3.1E-06 | 3.6E-02 | 2.3E-02 | 3.3E-03 | 9.3E-03 |
| 1.84E+04 | 1.4E-07 | 3.80E-07 | 6.10E-01 | 3.3E-07 | 2.3E-07 | 2.9E-03 | 1.8E-03 | 2.3E-04 | 6.3E-04 |
| 2.30E+04 | 5.2E-09 | 1.58E-08 | 6.48E-01 | 1.2E-08 | 9.0E-09 | 1.2E-04 | 7.5E-05 | 8.7E-06 | 2.2E-05 |
| 2.87E+04 | 8.8E-11 | 2.95E-10 | 6.83E-01 | 2.0E-10 | 1.6E-10 | 2.4E-06 | 1.4E-06 | 1.5E-07 | 3.5E-07 |
| 3.59E+04 | 5.6E-13 | 2.04E-12 | 7.15E-01 | 1.3E-12 | 1.0E-12 | 1.7E-08 | 9.8E-09 | 9.0E-10 | 2.1E-09 |
| 4.48E+04 | 1.0E-15 | 4.07E-15 | 7.44E-01 | 2.2E-15 | 1.8E-15 | 3.4E-11 | 1.9E-11 | 1.6E-12 | 3.5E-12 |
| 5.61E+04 | 3.8E-19 | 1.72E-18 | 7.70E-01 | 8.5E-19 | 7.1E-19 | 1.5E-14 | 8.2E-15 | 6.1E-16 | 1.3E-15 |
| 7.01E+04 | 2.1E-23 | 1.04E-22 | 7.94E-01 | 4.6E-23 | 3.9E-23 | 8.9E-19 | 5.0E-19 | 3.3E-20 | 6.5E-20 |
| 8.76E+04 | 1.0E-28 | 5.55E-28 | 8.15E-01 | 2.2E-28 | 1.9E-28 | 4.8E-24 | 2.7E-24 | 1.6E-25 | 3.0E-25 |
| 1.09E+05 | 2.3E-35 | 1.42E-34 | 8.34E-01 | 5.0E-35 | 4.4E-35 | 1.2E-30 | 6.8E-31 | 3.6E-32 | 6.5E-32 |
| 1.37E+05 | 1.2E-43 | 8.21E-43 | 8.52E-01 | 2.6E-43 | 2.3E-43 | 7.3E-39 | 3.9E-39 | 1.9E-40 | 3.2E-40 |
| 1.71E+05 | 5.4E-54 | 4.13E-53 | 8.67E-01 | 1.2E-53 | 1.1E-53 | 3.7E-49 | 2.0E-49 | 8.3E-51 | 1.4E-50 |
| 2.14E+05 | 6.5E-67 | 5.52E-66 | 8.81E-01 | 1.4E-66 | 1.3E-66 | 5.0E-62 | 2.6E-62 | 1.0E-63 | 1.6E-63 |
| 2.67E+05 | 4.7E-83 | 4.47E-82 | 8.94E-01 | 1.0E-82 | 9.3E-83 | 4.1E-78 | 2.1E-78 | 7.2E-80 | 1.1E-79 |
| 3.34E+05 | 3.3E-103 | 3.44E-102 | 9.05E-01 | 6.9E-103 | 6.4E-103 | 3.1E-98 | 1.6E-98 | 5.0E-100 | 7.4E-100 |
| 4.18E+05 | 2.1E-128 | 2.47E-127 | 9.15E-01 | 4.5E-128 | 4.2E-128 | 2.3E-123 | 1.2E-123 | 3.2E-125 | 4.6E-125 |
| 5.22E+05 | 7.0E-160 | 9.20E-159 | 9.24E-01 | 1.5E-159 | 1.4E-159 | 8.5E-155 | 4.4E-155 | 1.1E-156 | 1.5E-156 |
| 6.53E+05 | 3.2E-199 | 4.76E-198 | 9.32E-01 | 6.9E-199 | 6.5E-199 | 4.4E-194 | 2.3E-194 | 4.9E-196 | 6.7E-196 |
| 8.16E+05 | 2.3E-248 | 3.71E-247 | 9.39E-01 | 4.8E-248 | 4.6E-248 | 3.4E-243 | 1.8E-243 | 3.4E-245 | 4.6E-245 |
| 1.02E+06 | 0.0E+00 | 0.00E+00 | 9.45E-01 | 0.0E+00 | #NUM! | 1.4E-304 | 7.3E-305 | 1.3E-306 | 1.6E-306 |