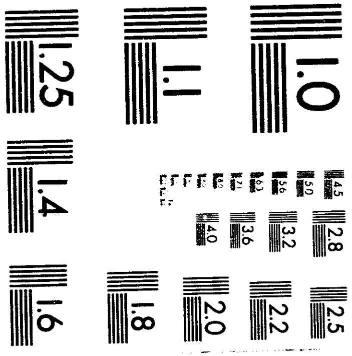
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Performance Assessment of the Greater Confinement Disposal Facility on the Nevada Test Site: Comparing the Performance of Two Conceptual Site Models*

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ABSTRACT

A small amount of transuranic (TRU) waste has been disposed of at the Greater Confinement Disposal (GCD) site located on the Nevada Test Site's (NTS) Radioactive Waste Management Site (RWMS). The waste has been buried in several deep (37 m) boreholes dug into the floor of an alluvial basin. For the waste to remain in its current configuration, the DOE must demonstrate compliance of the site with the TRU disposal requirements, 40 CFR 191. Sandia's approach to process modelling in performance assessment is to use demonstrably conservative models of the site. Choosing the most conservative model, however, can be uncertain. As an example, diffusion of contaminants upward from the buried waste in the vadose zone water is the primary mechanism of release. This process can be modelled as straight upward planar diffusion or as spherical diffusion in all directions. The former has high fluxes but low release areas, the latter has lower fluxes but is spread over a greater area. We have developed analytic solutions to a simple test problem for both models and compared the total integrated discharges. The spherical diffusion conceptual model results in at least five times greater release to the accessible environment than the planar model at all diffusivities. Modifying the planar model to allow for a larger release, however, compensated for the smaller original planar discharge and resulted in a new planar model that was more conservative that the spherical model except at low diffusivities.

GENERAL INFORMATION

Description of Facility

The Greater Confinement Disposal (GCD) facility is located within the Radioactive Waste Management Site (RWMS) at the Nevada Test Site (NTS). The facility consists of several boreholes, 3 to 3.7 m in diameter and 37 m in depth, augured into the alluvial fill of an aggrading basin in southern Nevada known as Frenchman Flat. Various articles that have been contaminated with isotopes of depleted and enriched uranium and plutonium was distributed amonst four of these boreholes, and each was backfilled completely with 22 m of sifted alluvium. A small berm on each borehole was constructed to allow for settling.

Alluvium fills the basin to a depth of approximately 460 m. The nearest groundwater is an unconfined aquifer some 235 m below the surface. The vegetation overlying the facility is

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DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED characteristic of the Northern Mojave desert, typically dominated by *Larrea Tridentata* (creosote). The site is highly arid with rainfall averaging only about 13 cm per year, which when combined with a high evapotranspiration potential, serves to limit the magnitude of the downward recharge rate. Based upon environmental tracer data, Conrad[1] concluded that for current climatic conditions the downward recharge rate was not great enough for radionuclides to be convected to the unconfined aquifer in a period of 10,000 years. Consequently under current conditions, the only pathway for release in 10,000 years is diffusion of dissolved radionuclides upwards to the surface in the vadose zone water.

Performance Measure - 40 CFR 191

Disposal of transuranic (TRU) waste must be in accordance with 40 CFR 191, the standard established by the EPA in 1985.[2] This regulation consists of three primary quantitative requirements, (1) the Containment Requirements, (2) the Individual Protection Requirements, and (3) the Groundwater Protection Requirements. It is within the context of these requirements that we determine the performance of any TRU disposal site. The intent of this paper is not to conduct a total system performance assessment of the GCD site, but rather to compare the performance of two different contaminant transport conceptual models of the site. In addition, we have restricted our attention to just the Containment Requirements. These requirements restrict the probability that the total integrated discharge of radioactivity to the "accessible environment" over a period of 10,000 years will not exceed specified limits. The total integrated discharge will therefore be the performance measure on which we will base our comparison of the two concepual models of the site. Within the context of the two models to be discussed below, the accessible environment refers only to the land surface above the waste facility.

Modelling Approach

Modelling is the only practical means by which the total integrated discharge can be determined over a period of 10,000 years. However, the large time and distance scales involved in modelling the site are such that we must admit that development of a realistic model of the site is an impossibility. The actual release from the site can never be accurately predicted. It is still possible to assess site safety, however, if that assessment is based upon conservative models. That is, models that consistently overpredict the release in relation to what the actual release would be. If it can be shown that the conservative model complies with the regulations, it therefore follows that the site itself should also comply.

However, since the actual release cannot be determined, it is difficult to show that a given model is truly conservative. We assume that if at each step of the model development, a consistent conservative bias is introduced the end result will be a conservative model. The judgement of the analyst must be relied upon to a large extent in making these choices. Unfortunately, because of the intricacies of the system, it may be difficult to choose between two or more conceptual site models on the basis of subjective judgement or heuristic arguments alone. The only recourse at this point is to perform an assessment analysis using each conceptual model in turn. Comparision of the results should resolve which conceptual model should be used to achieve a conservative result.

In this paper, we present one such comparision of conceptual models of the GCD site. In the current conceptualization of the site, the fact that the recharge rate is relatively small implies that the primary mechanism for release is diffusion of dissolved radionuclides upwards in the unsaturated zone pore water until they either reach the surface or are absorbed into plants and subsequently transported into the accessible environment. At issue is the nature (*i.e.*, geometry) of this diffusion. The simplest picture is to imagine that diffusion will occur in one-dimension only, that is, straight upwards through an isotropic, homogeneous alluvium backfill to the surface with no lateral dispersion, governed by a planar diffusion operator. This presents the shortest average path to the accessible environment as well as relatively high fluxes. Thus, it would seem to also be the most conservative picture. An alternative conceptualization is that diffusion occurs radially outward in three dimensions in accordance with a spherical diffusion operator. Generally speaking, this alternative conceptualization will have lower fluxes at a given distance from the source and involve a greater average pathlength to the surface. Thus, it would appear that the spherical diffusion conceptualization is not as conservative as the planar diffusion conceptualization. On the other hand, spherical diffusion will discharge radionuclides over a much greater area than the planar conceptualization. This greater area might offset the smaller fluxes and greater travel times so that the spherical diffusion conceptualization would actually result in the higher releases. This question cannot be resolved, however, unless recourse is made to an actual analysis of the two conceptualizations. It should also be noted that other conceptual models are possible, for example, inclusion of a layering in the alluvium. These, however, require their own analysis and will not be considered in this study.

PLANAR DIFFUSION MODEL

This conceptual model of release assumes that radionuclides will dissolve into the unsaturated zone liquid phase in the source area. They will then diffuse straight upwards, remaining confined to the cylinder of alluvium that overlies the borehole. Species will decay as

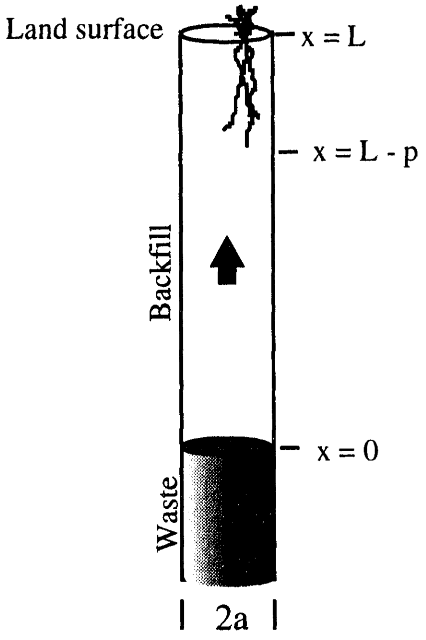

Figure 1 - Planar Diffusion Model

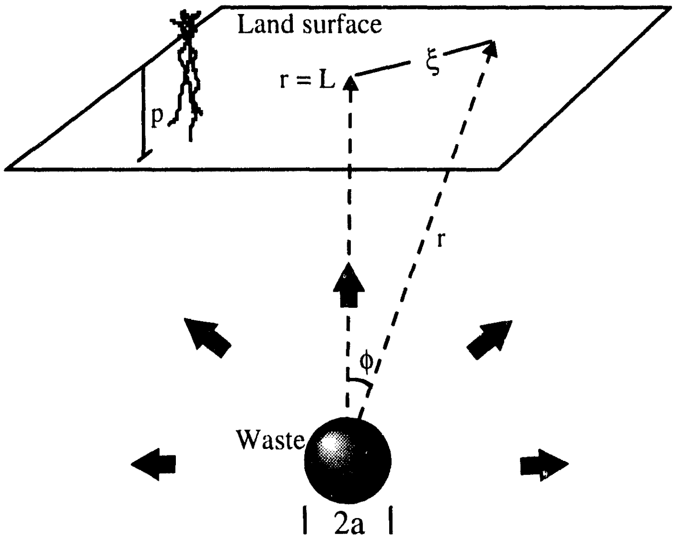

Figure 2 - Spherical Diffusion Model

they diffuse and will also adsorb onto the surrounding alluvium as determined by the commonly used distribution coefficient, K_d. Upon reaching the root zone, a distance *p* below the surface, some radionuclides may be absorbed by plants and transported directly to the surface. Radionuclides that diffuse all the way to the surface are dispersed so that they do not accumulate at the surface. This conceptual model is depicted in Figure 1.

For this analysis, we restrict our attention to transport of a single parent species. The mathematical representation of the planar conceptual model is as follows [3]:

$$\frac{\partial C}{\partial t} = \frac{D}{\tau R}\frac{\partial^2 C}{\partial x^2} - \lambda C \,, \tag{1}$$

where

$$R = 1 + \frac{\rho K_d}{\theta} \tag{2}$$

$C(x,t)$ = concentration of the radionuclide, [g/m^3]
D = free-water molecular diffusion coefficient, [m^2/yr]
τ = convolusion factor, a factor always greater than one which represents the degree to which diffusion is slowed by the porous media.[dimensionless]
λ = radioactive decay constant, [yr^{-1}]
K_d = distribution coefficient of a linear sorption model [m^3/kg]
θ = unsaturated moisture content, [dimensionless]
ρ = bulk density of alluvium, [kg/m^3].

The problem extends over a domain from x = 0 at the top of the buried waste to x = L at the surface. At the source, we established a constant essential condition, which presumes that there is enough solid waste present that the liquid phase concentration will be maintained at its solubility limit. At the surface, the radionuclides are dispersed so that the concentration will remain zero at that point. This condition is a conservative choice because it ensures the largest average driving force for diffusive mass transfer. Finally, we assume that there is initially no contamination outside of the source area. These conditions on the problem are expressed as,

$$C(0,t>0) = C_0, \quad C(L,t) = 0, \quad C(x,0) = 0 \tag{3}$$

where C_0 is the solubility limit of the species.

An analytical solution can be obtained to this problem. We find that,

$$\begin{aligned} C(x,t) = \frac{C_0}{2}\sum_{n=0}^{\infty}\Bigg(& \exp\left(-(2nL+x)\sqrt{\frac{\lambda}{D_e}}\right) erfc\left[\frac{2nL+x}{\sqrt{4D_e t}} - \sqrt{\lambda t}\right] + \exp\left((2nL+x)\sqrt{\frac{\lambda}{D_e}}\right) erfc\left[\frac{2nL+x}{\sqrt{4D_e t}} + \sqrt{\lambda t}\right] \\ & - \exp\left(-(2(n+1)L-x)\sqrt{\frac{\lambda}{D_e}}\right) erfc\left[\frac{2(n+1)L-x}{\sqrt{4D_e t}} - \sqrt{\lambda t}\right] - \exp\left((2(n+1)L-x)\sqrt{\frac{\lambda}{D_e}}\right) erfc\left[\frac{2(n+1)L-x}{\sqrt{4D_e t}} + \sqrt{\lambda t}\right]\Bigg) \end{aligned} \tag{4}$$

where D_e, the effective diffusivity, is defined as,

$$D_e = \frac{D}{\tau R} \tag{5}$$

The release flux at the surface is obtained by a simple application of Fick's first law [4],

$$|j_{surf}| = -\frac{\theta D}{\tau}\frac{\partial C}{\partial x}\bigg|_{x=L} \tag{6}$$

Absorption of radionuclides into plants is modelled through use of a parameter known as the concentration ratio. It is the ratio between the specific activity in the above ground tissues of plants grown in contaminated soil and the specific activity within the contaminated soil. It is defined as,

$$CR = \frac{Ci/g \text{ dry above ground vegetation}}{Ci/g \text{ dry soil}} \tag{7}$$

If the depth of the root zone is assumed to be a constant distance below the surface and the vegetation is assumed to regenerate completely on a yearly basis, then it is possible to show[5] that the flux through the vegetative pathway is given by,

$$|j_{veg}| = \alpha B\ CR\left(\frac{\theta}{\rho}+K_d\right)C(L-p,t) \tag{8}$$

where

B = above ground standing biomass density (kg/m^2)
α = number of times the standing biomass B is turned over in a year
p = depth of the root zone (m).

From the surface and vegetative flux values, we can determine the total integrated discharge in 10,000 years:

$$Q = \int_0^{10,000} A(\,|j_{surf}| + |j_{veg}|\,)\,dt \tag{9}$$

where $A = \pi a^2$. Note that the release area is confined to just the borehole cross-section.

SPHERICAL DIFFUSION MODEL

The spherical diffusion conceptual model differs from the planar diffusion model only to the extent that radionuclides are now allowed to diffuse away from the source in all directions. Also for purposes of mathematical tractibility, we assume the original waste is confined to a sphere of radius a buried a depth L below the surface. This new conceptual model as well as the spherical coordinate system associated with it is depicted in Figure 2.

The differential equation that governs diffusion, retardation, and decay in a spherical geometry is as follows [4],

$$\frac{\partial C}{\partial t} = \frac{D}{\tau R}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial C}{\partial r}\right) + \frac{1}{r^2 \sin\phi}\frac{\partial}{\partial \phi}\left(\sin\phi \frac{\partial C}{\partial \phi}\right)\right] - \lambda C \tag{10}$$

At the surface of the sphere surrounding the waste, we assign a constant concentration equal to the solubility limit. As before, a zero concentration condition is established at the ground surface, which in the present coordinate system is a surface defined by $r\cos\phi = L$. The initial condition is identical to the planar model. Symbolically, these conditions are,

$$C(a,\phi,t>0) = C_0,\ C(r\cos\phi = L,t) = 0,\ C(r,\phi,0) = 0. \tag{11}$$

The presence of the ground surface constraint complicates finding a solution to this problem. Carslaw and Jaeger [6] give a solution for diffusion from a sphere into an infinite unconstrained medium. We can use this rudimentary solution to develop a solution to the constrained problem through the use of the method of images, an established procedure in well drawdown computations .[3] We obtain,

$$\begin{aligned} C(r,\phi,t) = \frac{aC_0}{2r}\sum_{n=0}^{\infty}\Bigg(& \exp\left(-(r_{+n}-a)\sqrt{\frac{\lambda}{D_e}}\right) erfc\left[\frac{r_{+n}-a}{\sqrt{4D_e t}} - \sqrt{\lambda t}\right] + \exp\left((r_{+n}-a)\sqrt{\frac{\lambda}{D_e}}\right) erfc\left[\frac{r_{+n}-a}{\sqrt{4D_e t}} + \sqrt{\lambda t}\right] \\ & - \exp\left(-(r_{-n}-a)\sqrt{\frac{\lambda}{D_e}}\right) erfc\left[\frac{r_{-n}-a}{\sqrt{4D_e t}} - \sqrt{\lambda t}\right] - \exp\left((r_{-n}-a)\sqrt{\frac{\lambda}{D_e}}\right) erfc\left[\frac{r_{-n}-a}{\sqrt{4D_e t}} + \sqrt{\lambda t}\right]\Bigg) \end{aligned} \tag{12}$$

where

$$\begin{aligned} r_{+n}^2 &= r^2 + (2nL)^2 + 4nLr\cos\phi \\ r_{-n}^2 &= r^2 + (2(n+1)L)^2 - 4(n+1)Lr\cos\phi \end{aligned} \tag{13}$$

We note that Eq. (12) is not an exact solution because it predicts a concentration at the source which is slightly different from C_0. However, for the time scales and values of diffusivity used here, this discrepancy will be at most 0.25%.

Obtaining the surface flux from this expression is also more complicated than in the planar model. We must first introduce the surface coordinate, ξ, which is the horizontal distance away from the vertical line that passes through the center of the waste as depicted in Figure 2. Now, we note that the flux vector is given by the expression,

$$\vec{j} = -\frac{\theta D}{\tau}\nabla C \tag{14}$$

Hence, the magnitude of the flux leaving the surface is obtained by the following,

$$|j_{surf}| = \vec{j}\cdot\vec{n} = -\frac{\theta D}{\tau}\left[\frac{L}{(L^2+\xi^2)^{1/2}}\frac{\partial C}{\partial r} - \frac{\xi}{L^2+\xi^2}\frac{\partial C}{\partial \phi}\right] \tag{15}$$

where $\vec{n}$ is the unit normal vector pointing upward out of the ground surface.

The release flux through the plant pathway is obtained by computing the concentration on the parallel plane that is *p* meters below the ground surface. This plane satisfies the constraining equation $r \cos \phi = L - p$. Thus, the vegative flux is given by,

$$|j_{veg}| = \alpha B \; CR \left(\frac{\theta}{\rho} + K_d\right) C(r\cos\phi = L - p, t) \tag{16}$$

Finally, the total integrated discharge is obtained by integration across the entirety of the ground surface and over a period of 10,000 years.

$$Q = \int_0^{10,000} \int_0^{\infty} 2\pi\left(|j_{surf}| + |j_{veg}|\right) \xi \, d\xi \, dt \tag{17}$$

COMPARING TOTAL INTEGRATED DISCHARGE OF BOTH MODELS

The expressions developed for total integrated discharge developed in the previous two sections were used to evaluate the relative discharge of both conceptual models for a number of different model parameter combinations. Some of the parameters, however, have little uncertainty or did not affect the results to a great extent and were kept at fixed values. The molecular diffusion coefficient, D, was maintained at 0.0315 m^2/yr. This value is reasonable for most species in aqueous solution. The depth of burial, L, was fixed at 19.3 m, which allows for the possibility that erosional process might remove 2 m of the original 21.3 m of backfill. The radius of both the cylindrical and spherical source areas was held at 1.5 m. The rooting depth was fixed at 10.7 m, thought to be a very conservative value of rooting depth for Frenchman Flat. The biomass density was set at 0.49 kg/m^2, a value characteristic of actual Frenchman Flat vegetation communities .[7] It was assumed that the entire standing biomass would be turned over twice in a year's time; that is, α would equal 2. Finally, the species half-life, solubility limit, and concentration ratio were set at 30,000 years, 0.25 mg/kg, and 0.002 Ci/g plant/ Ci/g soil, respectively. These values are roughly representative of Pu-239. There is no need to use conservative values for these latter parameters since each has approximately the same affect on the discharge from both models.

The remaining parameters (the convolusion factor, the moisture content, and the adsorption coefficient, K_d) have a direct effect on the effective diffusivity, D_e, which is the key parameter controlling the release. They were varied in order to obtain different values of effective diffusivity. These values appear in Table 1 along with the corresponding effective diffusivity and the total integrated discharge in grams for each conceptual model. The latter two values were obtained by numerical integration of Eqs. (9) and (17) above. Simpson's rule on a uniform grid was used for each integral. In the case of the spatial ξ integration , the integration was carried out only to ξ=50 m since contribution to the total at greater distances amounted to at most 0.02% of the total.

The results for effective diffusivities that range from 10^{-2} to roughly 9 x 10^{-5} m^2/yr are shown in Table 1. For diffusivities less than 5 x 10^{-5} m^2/yr the predicted discharge from each model amounts to atoms or fractions of atoms. We chose not to draw conclusions in this range of diffusivity. The last column of Table 1 lists the ratio of the total integrated discharge associated with the spherical conceptual model to the like quantity computed for the planar

Run	τ	θ	K_d (cm^3/g)	D_e (m^2/yr)	Total Integrated Discharge (g)		Ratio of Spherical to Planar
					Planar Model	Spherical Model	
1	3	0.18	0.001	1.04×10^{-2}	0.71	5.8	8.2
2	6	0.18	0.001	5.20×10^{-3}	0.13	0.83	6.3
3	15	0.18	0.001	2.08×10^{-3}	3.0×10^{-3}	1.5×10^{-2}	5.2
4	36	0.18	0.015	7.73×10^{-4}	2.5×10^{-5}	1.4×10^{-4}	5.5
5	45	0.18	0.084	4.03×10^{-4}	2.0×10^{-6}	1.5×10^{-5}	7.4
6	26	0.15	1.0	1.07×10^{-4}	5.2×10^{-12}	8.6×10^{-10}	170
7	57	0.18	0.61	8.68×10^{-5}	4.7×10^{-14}	2.4×10^{-11}	507

Table 1 - Ratio of spherical to planar discharge as a function of diffusivity

model. In all cases, the spherical discharge is at least five times larger than the planar discharge with the ratio increasing rapidly as the effective diffusivity decreases. Thus, we are led to the conclusion that, although the flux vector in the spherical model is generally much smaller than in the planar model, the larger area that the spherical model affects more than compensates for the smaller flux. It appears clear that the spherical diffusion model is the more conservative representation of diffusive transport at the GCD facility.

APPLYING TIME-VARIANT AREA TO THE PLANAR MODEL

This last result is rather inconvenient. Because of the necessity of considering the decay of chains of radionuclides each with its own effective diffusivity in the actual performance assessment, applying the spherical model to the actual performance assessment of the site would require two- or possibly three- dimensional numerical modelling. This is undesirable because we must use a Monte Carlo technique to address the uncertainty in system. In this context, using complex numerical models is very expensive and time-consuming. It would better if we could retain the relative simplicity of the planar model but alter it so that its discharge would be larger than the corresponding spherical model.

One possibility is to allow the discharge area that multplies the planar flux values to be larger than the borehole cross-section. The spherical diffusion model suggests that the affected area will start small and grow with time as the spherical diffusion "front" spreads outwards from the source and intersects the ground surface. Within this area the majority of the release occurs. We might use a similar idea in determining the discharge area for the planar model. We propose the following function for this area,

$$A(t) = \begin{cases} \pi a^2 \ ; \ \xi^*(t) \le a \\ \pi(\xi^*(t))^2 \ ; \ \xi^*(t) > a \end{cases} \tag{18}$$

where

$$\xi^*(t) = \sqrt{(R^*)^2 - L^2} \ ; \ R^* = 2\sqrt{4D_e t}$$

Thus, $\xi^*(t)$ is the expanding radius of the discharge area and R^* is the hypotenuse of a cone with apex at the waste which subtends the discharge area. We have made R^* twice the diffusion length scale, $\sqrt{4D_e t}$, so it approximately represents the extent to which the spherical diffusion "front" has spread away from the waste area. This area computation is depicted in Figure 3.

The area computed by Eq. (18) is used instead of πa^2 in Eq. (9) when computing the total integrated discharge for the planar model. The ratio of the discharge from the spherical model to that for the planar model using this "conical" area for several different effective diffusivities is shown in Table 2. We see now that using a time dependent area results in the planar model having the largest discharges, except for diffusivities less than about 10^{-4} m^2/yr. It can be argued[3] that the compliance of the site will not be affected to a significant degree by situations with diffusivities smaller than 10^{-4} m^2/yr . Consequently, using the planar conceptual model with the time-dependent discharge area would result in the most conservative answer in the context of judging the compliance of the site.

D_e (m^2/yr)	1.04×10^{-2}	5.20×10^{-3}	2.60×10^{-3}	1.04×10^{-3}
Ratio of Spherical to Planar Model using "conical area"	0.02	0.05	0.81	5.5

Table 2 - Ratio of spherical to planar discharge using conical area alteration

SUMMARY AND CONCLUSIONS

One of the chief difficulties with using conservative models for performance assessment is that it can sometimes be difficult to judge *a priori* which conceptual model of a site will result in the worst site performance. The only recourse in this situation is to consider the performance of the site with respect to both models. The model that results in the worst performance is the most conservative model within the set of those considered.

In this paper, we have considered one example of this procedure. The lack of downward recharge at the GCD implies that release of radionuclides can occur only by diffusion upwards in the vadose zone water. We have considered two conceptual models of this diffusion, planar and spherical. We developed analytical solutions of both models for the simple problem of a single diffusing parent species. A comparison of the total integrated discharge determined from both of these solutions showed that the spherical model was consistently more conservative than the planar model. We took our analysis one step further by altering the planar diffusion model so that the affected area would expand with time in a manner suggested by the spherical conceptual model. In the latter case, we found that the altered planar model would result in the highest release at high diffusivities, but the spherical model would become more conservative at lower values. Since the compliance of the site was more dependent upon high diffusivity situations, we felt justified in concluding that the altered planar model would be the most conservative model among those considered in this paper. Other conceptual models exist. The presence of layered structures in the alluvium is an example. Evaluating these other models, however, was beyond the scope of this paper.

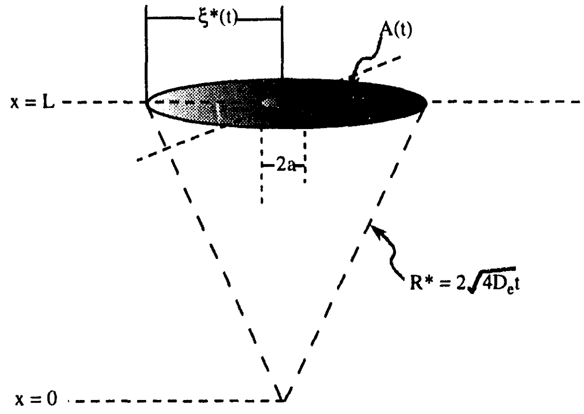

Figure 3 - Sketch of conical area approach

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