VERIFICATION DOCUMENT
FOR
HWIR99 LANDFILL MODULE

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ACKNOWLEDGMENTS

A number of individuals have been involved with the verification of the landfill module. Dr. Zubair A. Saleem of the U.S.EPA, Office of Solid Waste, provided overall technical coordination and review throughout this work. Dr. Varut Guvanasen of HydroGeoLogic, Inc. developed the reactor type solution and the one-dimensional transport solution without the landfill cover to verify the Landfill Module. Mr. Patrick Sullivan of HydroGeoLogic, Inc. performed the module runs and the verification of the emission fluxes. The report was prepared by Dr. V. Guvanasen and Mr. P. Sullivan.

1.0 BACKGROUND

A landfill unit, as simulated by the HWIR-3MRA Landfill Module (LM) (RTI, 1999), consists of a number of landfill cells. A landfill cell comprises three components from top to bottom: landfill cover, waste, and landfill liner (or subsoil). The landfill consists of a number of cells, each cell taking approximately one year to fill to its capacity. Each cell is left exposed during the first year (waste emplacement period) and the cover is placed on the cell at the end of the year.

A semi-analytical reactor type model (SAM) was developed for comparing with LM. SAM was used as an interim reference to provide bounds of physical behaviors of contaminant migration from landfills.

The verification plan, and software and data sources are outlined in Sections 2 and 3. SAM is described in Section 4. Verification results are presented in Section 5. Calculations relating to the verification are presented in Appendix A.

After the completion of this verification document, additional changes were made to LM. Comments on the results of the new LM are presented in Appendix B.

2.0 VERIFICATION PLAN

The verification was divided into two stages, described below:

Stage 1	Verification of two predominant contaminant mass fluxes: the leachate mass flux and the volatile emission flux, assuming that the particulate emission flux was correct and the degradation was absent.
Stage 2	Verification of the remaining components.

The verification was conducted using information from the SSF and GRF files for Setting LF 223 504.

3.0 SOFTWARE VERIFIED AND DATA USED

The LM is written in Microsoft Visual C++, Version 6.0. The first version of LM source code and documentation (RTI, 1999) were received on April 18, 1999. A number of verification runs were conducted and a number of technical issues were raised. In response to the technical issues, the module was modified with a number of changes incorporated. The second version of LM was received on May 25, 1999. One of the changes was the by-pass of the subsoil or landfill liner.

Runs with both zero and non-zero subsoil thicknesses were conducted. For the latter, the source code was altered to include the subsoil to demonstrate the effects that the subsoil may have on concentration of the contaminant as it migrates through the subsoil.

The verification was conducted using information from the SSF and GRF files for Setting LF 223 504. For this setting, all the degradation rate constants (biodegradation, hydrolysis, etc.) in the input files provided were zero.

Runs of the landfill module were conducted using the properties of benzene. Alternative runs with dioxin yielded no leachate concentration.

4.0 SEMI-ANALYTICAL SOLUTION

A semi-analytical reactor type model (SAM) was developed for comparing with LM. SAM is based on the following assumptions:

- Each cell is capped with landfill cover with from the very beginning
- There is no liner. (Transport in the liner is steady state with no time lag.)
- Transport in the landfill cover is steady state and is only diffusional
- Particulate emission is negligible.

The processes simulated in SAM may not correspond exactly with those in the LM. However, the time frame of the transport problem is so large with the transport occurring so slowly that the above assumptions are reasonably justified in most cases. SAM was used as an interim reference to provide bounds of physical behaviors of contaminant migration from landfills.

The semi-analytical solution is provided below.

In a given cell, the following mass balance equation may be written:

$$\frac{dM_j}{dt} = -A_j I C_{Lj} - ((1-\theta)\rho_s K_d + \theta S_w)\lambda V_j C_{Lj} - \theta_{cov} S_{acov} D_{acov} H' C_{Lj} \frac{A_j}{L_{cov}} \qquad \textbf{(1)}$$

where

M_j = Total contaminant mass in Cell j at time t

= $((1-\theta)\rho_s K_d + \theta S_w + H'\theta S_a) V_j \; C_{Lj}$

t = Time
A_j = Base area of Cell j
C_{Lj} = Leachate contribution from Cell j
I = Infiltration rate
H' = Henry's constant
V_j = Volume occupied by Cell j
θ = Porosity of the waste
θ_{cov} = Porosity of landfill cover
L_{cov} = Thickness of landfill cover
S_w = Water saturation of the waste
S_a = Air saturation of the waste
S_{acov} = Air saturation in landfill cover
D_{acov} = Effective diffusion coefficient for benzene in landfill cover

$$= \frac{(\theta_{cov} S_{acov})^{\frac{7}{3}} D_a}{\theta_{cov}^2}$$

D_a = Molecular benzene diffusivity in air.

Solving Equation (1) based on the initial condition of $C_{Lj} = C_{Lj}^o$ at the beginning of operation, one obtains:

$$C_{Lj} = C_{Lj}^{o} \exp(-\kappa t) \qquad \textbf{(2)}$$

where

t = Time from the beginning of the placement in the cell (years)

$$\kappa = \frac{A_j I + ((1-\theta)\rho_s K_d + \theta S_w)\lambda V_j + \theta_{cov} S_{acov} D_{acov} H' \frac{A_j}{L_{cov}}}{((1-\theta)\rho_s K_d + \theta S_w + H'\theta S_a) V_j}$$

Summing contributions from all the landfill cells, one obtains:

$$C_{Lave} = \frac{\sum_{j=1}^{n_{Cells}} A_j C_{Lj}(t-j+1)}{\sum_{j=1}^{n_{Cells}} A_j} \qquad \textbf{(3)}$$

where

C_{Lave} = Annual average leachate concentration for the whole landfill
$C_{Lj}(m)$ = Leachate concentration for Cell j at time m years
= 0, if $m < 0$.
n_{Cells} = Number of landfill cells

Annual average leachate flux per unit area, F_{LA}, is approximated by:

$$F_{LA} = I C_{Lave} \qquad \textbf{(4)}$$

Annual average volatile emission flux per unit area is approximated by:

$$F_{VEA} = D_{acov} H' S_{acov} \theta_{cov} \frac{C_{Lave}}{L_{cov}} \tag{5}$$

5.0 RESULTS

5.1 Background

- The landfill of interest has 25 cells. It takes one year for a cell to come on line (or to be fully emplaced), and therefore 25 years to have all cells as leachate generators.

- Three cases were of interest. Runs with typical K_{oc} (53 ml/g), and low and high K_{oc}'s (0.53 and 5,300 ml/g, respectively) were conducted.

- Runs with two liner thicknesses (1.4 m and 0 m) were conducted.

5.2 Results

Time-varying leachate fluxes in (g/m^2/d) at the bottom of the liner in the case of non-zero liner thickness, and at the bottom of the waste in the case of zero liner thickness, are shown in Figures 1a, 1b, and 1c, for the cases of low, typical (for benzene), and high K_{oc} values, respectively. Corresponding volatile emission fluxes are shown in Figures 2a, 2b, and 2c, respectively.

The following problems are highlighted:

- Simulations of the LM were terminated at 200 years or less. In many cases, effluxes from the landfills are still significant at 200 years.

- Physically impossible leachate concentration in the liner.

  In Figure 1b, one can see that the leachate concentration is higher than the leachate concentration at the bottom of the liner (Zs = 1.4 m) is greater than the leachate concentration at the bottom of the waste (Zs = 0.0 m with the liner by-passed). (Zs is the thickness of the liner.) Note also that the peak concentration in the case of non-zero liner thickness is almost twice the equilibrium aqueous concentration, (see Table 1). This irregularity may be attributed to the imposed condition of mass balance at the interface between the liner and the waste, or the condition of continuity of leachate concentration described in Section 6.

  In the case of high K_{oc}, the generation of leachate concentration may be incorrect. See Figure 1c. The leachate concentration at the bottom of the waste during the first 100 years is zero, while the leachate concentration at the bottom of the liner is greater than zero. This is physically unreasonable, and could be attributed to the interface conditions described in Section 6.

- Volatile emission flux may be too low.

For the SAM, the ratio of volatile emission and the leachate flux is obtained by dividing Equation (5) by Equation (4) to obtain:

$$\frac{\theta_{cov} S_{acov} D_a (S_{acov}\theta_{cov})^{\frac{7}{3}} H^{\prime}}{I L_{cov} \theta_{cov}^{2}} \qquad \textbf{(6)}$$

where

θ_{cov} = porosity of the landfill cover = 0.45
S_{acov} = air saturation = 0.4
L_{cov} = cover thickness = 1.38 m
D_a = air diffusivity of benzene = 138 m^2/ a
H' = Henry's constant = 0.14
I = infiltration rate = 0.956 m/ a

Using the above values of parameters:

Ratio = 0.23

Ratios were calculated at different times, as shown in Table 2, when near or pseudo steady state conditions are expected. As shown in Table 2, most of the ratios are well below the ratio at steady state. In the case of high K_{oc}, the ratio far exceeds the ratio at steady state. In this case the leachate flux is reported zero. Therefore, there is a possibility that the liner component may not be functioning properly.

Table 1 Leachate Concentration Based on Equilibrium Consideration K_{oc} = 53 ml/gm = 0.053 m^3/kg.

Description	Max Leachate Concentration (kg/m^3)	Max Leachate Flux at Peak (g/m^2/d) = 0.956/365 × 1000 C_{Lave}
Equilibrium Condition	2.27 × 10^{-6}	5.95 × 10^{-6}
SAM with 25 cells	2.16 × 10^{-6}	5.65 × 10^{-6}
LM with 25 cells at the bottom of the waste (Zs = 0.0 m)	2.30 × 10^{-6}(*)	6.03 × 10^{-6}
LM with 25 cells at the bottom of the liner (Zs = 1.4 m)	3.57 × 10^{-6}(*)	9.33 × 10^{-6}

Note

* Estimated using infiltration rate, diffusion flux is assumed insignificant due to small concentration gradient.

Table 2 Ratios of Volatile Emission Flux (g/m^2/d) to Leachate Flux (g/m^2/d) as Calculated using LM.

		RATIO	
Koc (mg/L)	Time (Year)	Liner thickness = 1.4 m	Liner thickness = 0 m
0.53	28	0.000 32	0.000 39
	36	0.000 012	0.000 017
53	26	0.054	0.077
	28	0.051	0.077
	200	0.003 3	0.003 1
5300	30	0.	Leachate flux not reported
	200	0.58	Leachate flux not reported

Note

Steady-state ratio = 0.23

6.0 COMMENTS ON THE INTERFACE CONDITIONS, SOLUTION ALGORITHM, AND FORMULATION

The solution scheme (RTI, 1999) adopted for the LM is similar to that of the method of characteristics (Huyakorn and Pinder, 1983) in which the transport equation is separated into different operators: convective, dispersive, and degradational. The method of characteristics tends to have problems associated with heterogeneous materials because of the difficulty in conserving mass across the interface. The comments below focus on the interface conditions and the problems that the solution algorithm may have at the interface.

6.1 Interface Conditions

The formulation is based on the total concentration, thus:

$$C_T = \rho_{HW} C_W f_{WMU} = K_{TL} C_L \tag{7}$$

where:

$$\begin{aligned} C_T &= (\rho_b f_{oc} K_{oc} + \theta S_w + \theta S_a H')C_L \\ K_{TL} &= \rho_b f_{oc} K_{oc} + \theta S_w + \theta S_a H' \end{aligned} \qquad \textbf{(8)}$$

C_T = Volume-based total waste concentration in all phases of a chemical (M/L^3)
C_W = Mass-based total waste concentration in all phases of a chemical (M/M)
C_L = Leachate concentration (M/L^3)
ρ_{HW} = Dry waste density (M/L^3)
θ = Porosity of the waste
S_w = Degree of saturation of water
S_a = Degree of saturation of air
ρ_b = Dry solid bulk density (M/L^3)
f_{oc} = Organic carbon fraction
f_{WMU} = Waste fraction
K_{oc} = Equilibrium partitioning coefficient normalized to organic carbon (L^3/ M)
H' = Henry's constant (unitless)

In the LM, the following boundary conditions are implemented for the homogeneous soil column:

a) At the upper boundary of soil column:

$$C_T = 0 \qquad \textbf{(9)}$$

b) At the bottom of the column, the condition varies between that in Equation (9) and :

$$\frac{\partial C_T}{\partial z} = 0 \qquad \textbf{(10)}$$

The condition in Equation (10) was used for the test problem.

The conditions at the interfaces between the waste and the landfill liner and between the waste and the landfill cover are not given in the document.

The following boundary conditions at the interface between two porous media is adapted from Bear (1972), and Baehr (1987):

$$\begin{aligned} C_{Lm} &= C_{Ln} \\ C_{am} &= C_{an} \end{aligned} \qquad (11)$$

$$\theta_m S_{wm} v_z C_m - \theta_m (S_{wm} D_{wm} + S_{am} D_{am} H^{\prime}) \frac{\partial C_{Lm}}{\partial z} = \theta_n S_{wn} v_z C_n - \theta_n (S_{wn} D_{wn} + S_{an} D_{an} H^{\prime}) \frac{\partial C_{Lm}}{\partial z} \quad (12)$$

where

C_{Li} = Aqueous concentration on Side i of the interface
C_{ai} = Vapor concentration on Side i of the interface
v_z = fluid velocity in the vertical (z) direction
D_{wi} = Diffusion coefficient in the aqueous phase on Side i of the interface in the z direction.
D_{ai} = Diffusion coefficient in the air phase on Side i of the interface in the z direction.
S_{wi} = Saturation in the aqueous phase on Side i of the interface
S_{ai} = Saturation in the air phase on Side i of the interface
θ_i = Porosity on Side i of the interface.

In the above list of variables, the subscript *i* takes on the values of either *n* or *m* and denotes the side of the interface of interest. Conditions in Equation (11) represent the continuity of aqueous and vapor concentrations. Condition in Equation (12) represents the continuity of mass flux. All the conditions in these two equations must be simultaneously observed. (*Note that mechanical dispersion is not included in the diffusion term in the LM. Justification for the omission of the mechanical dispersion should be included in the document.*)

In the LM, the above conditions may not be observed at interfaces between different materials.

6.2 Algorithm

The proposed solution method, based on the LM document, is based on a quasi-analytical approach that is a step-wise solution of the diffusion-convection-decay governing transport equation on the same computational grid. In essence, the method proceeds as follows:

- Diffusion step.
  The current mass in each grid block is allowed to be redistributed by diffusion for one time step.

- Decay step.
  The current mass, after redistribution by diffusion, is allowed to undergo decay for one time step.

- Convection step.
  At the end of the decay step, the current mass in each grid block is convected to the immediately down-gradient grid block.

See details in RTI (1999).

The method may have problems related to the transfer of mass across the interface between two different materials, as outlined below.

6.2.1 Convective Mass Transfer

As shown in Figure 3, the thicknesses of sub-layers (grid sizes) in the subsoil and waste zones are different (0.03 m in the waste zone vs. 0.02 m in the subsoil). In the document, it is not explicitly stated as to how the mass in the bottommost layer in the waste zone is convectively transferred to the top layer of subsoil in a mass conservative manner, while maintaining the condition of concentration continuity (Equations (11) and (12)). However, as stated in Section 2.4.2 of the LM document (RTI, 1999), "*All of the material in the bottom layer of the upstream zone will be carried into the top layer of the downstream zone after one-convection-based time step in the upstream zone*." As stated in the document, the time step, Δt, for a given zone is determined by $\Delta t = \Delta z / V_E$, where Δz is the grid size. In a homogeneous soil zone, this time step size would allow mass in an upstream pulse (which occupies one whole grid block) to move completely to the immediately downstream grid block. At the interface, the above condition can be written as:

$$(C_{Lu} K_{TLu}) \Delta z_u = (C_{Ld} K_{TLd}) \Delta z_d \tag{13}$$

where

C_{Lu} = Upstream aqueous concentration
C_{Ld} = Downstream aqueous concentration
K_{TLu} = Upstream partitioning constant defined in Equation (8)
K_{TLd} = Downstream partitioning constant defined in Equation (8)
Δz_u = Upstream grid size or layer thickness
Δz_d = Downstream grid size or layer thickness

In the above equation, the product in the parentheses is equivalent to the total concentration. One can readily see that if the upstream and downstream grid sizes are approximately equal and $K_{TLu} > K_{TLd}$, then $C_{TLu} < C_{TLd}$, which, apart from being physically impossible, violates the continuity condition in Equation (11).

In the test problem, at the waste-subsoil interface, as shown in Figure 3, the layer thickness in the waste zone ($\Delta z_u = 0.03$ m) is greater than the layer thickness in the subsoil ($\Delta z_d = 0.02$ m).

Based on the parameter values given in Appendix A, the following partitioning coefficients were calculated (see Appendix A): $K_{TLu} = 63.2$; and $K_{TLd} = 2.0$.

Using Equation (13), one can see that it is possible for aqueous concentration in the downgradient block could be much greater than the upgradient aqueous concentration. How the convective mass transfer is implemented at the interface is not explicitly shown in the document. If the mass in the bottommost layer in the waste is totally convectively transferred to the topmost layer in the subsoil (as shown in Equation (13)), it is possible also that the transferred mass could cause the concentration in the top layer of the subsoil is unrealistically high.

6.2.2 Diffusive Mass Transfer

The solution technique, according to the document (RTI, 1999), is based on the principle of superposition of diffusive contributions from pulses in all layers. The term diffusive mass transfer in this document includes two mass transfer in the aqueous and vapor phases (see the diffusive terms in Equation (12)).

As shown in Figure 4, at time t, square concentration pulses in Layer W_I in the waste zone and Layer SS_I in the subsoil are allowed to diffuse. The shapes of the diffused pulses are dictated by the magnitude of 'effective' dispersion coefficient, $D_E = D/K_{TL}$, where D is the phase-summed diffusivity and K_{TL} is previously defined. In general, K_{TL} in the waste zone is much greater than that in the subsoil zone (see previous subsection for example). Therefore the effective diffusion coefficent in the subsoil, D_{ESS}, is greater than the effective diffusion coefficient in the waste, D_{EW}. As shown in Figure 4, the diffusional spread in the subsoil could be much greater than the spread in the waste. After any given time period, Layer W_I could conceivably receive substantial mass contribution (through back diffusion) from Layer SS_I, while Layer SS_I receives little or no mass contribution from Layer W_I. In reality, the back diffusion from Layer SS_I can penetrate the waste zone very little because of the low effective diffusion coefficient in the waste zone (compare concentration profiles A and B in Figure 4) . The mass contribution to Layer W_I from Layer SS_I may be unrealistically too high, causing C_T (the total concentration) in Layer W_I to be greater than it should be. This may be partially responsible for the high concentration observed when the waste zone is underlain by a liner.

Using a similar line of reasoning, it can also be stated that back diffusion from the landfill cover is too great, making the volatile emission proportionally too small.

6.3 General Formulation

LM's formulation is based on the following assumptions:

- Isothermal flow and transport, and absence of thermal generation;
- Absence of effects due to geochemical conditions in landfill cells;
- Absence of gas generation within cells;
- Absence of convective cells resulting from gasification and heat generation; and
- Absence of barometrically induced flow.

Effects due to the omission of the above processes are not fully known. Additional studies should be done in the future to assess their impact on risk assessment.

7.0 SUMMARY

The HWIR Landfill Module (LM) was subject to a number of test cases for the verification of leachate and volatile emission fluxes, which are the two most prevalent fluxes for organic chemicals. A semi-analytical solution (SAM) was developed and was used as an interim reference to provide bounds of physical behaviors of contaminant migration from landfills. During the verification process, the following problems were uncovered:

- Termination of simulations of the LM at 200 years or less;
- Physically impossible leachate concentration in the subsoil (liner); and
- Possibly too low volatile emission flux.

The 2nd and 3rd problems could stem from the solution method and the way by which interfaces between different materials are treated. The problems are discussed in Section 5 and a discussion relating to the problems is presented in Section 6.

8.0 REFERENCES

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FIGURES

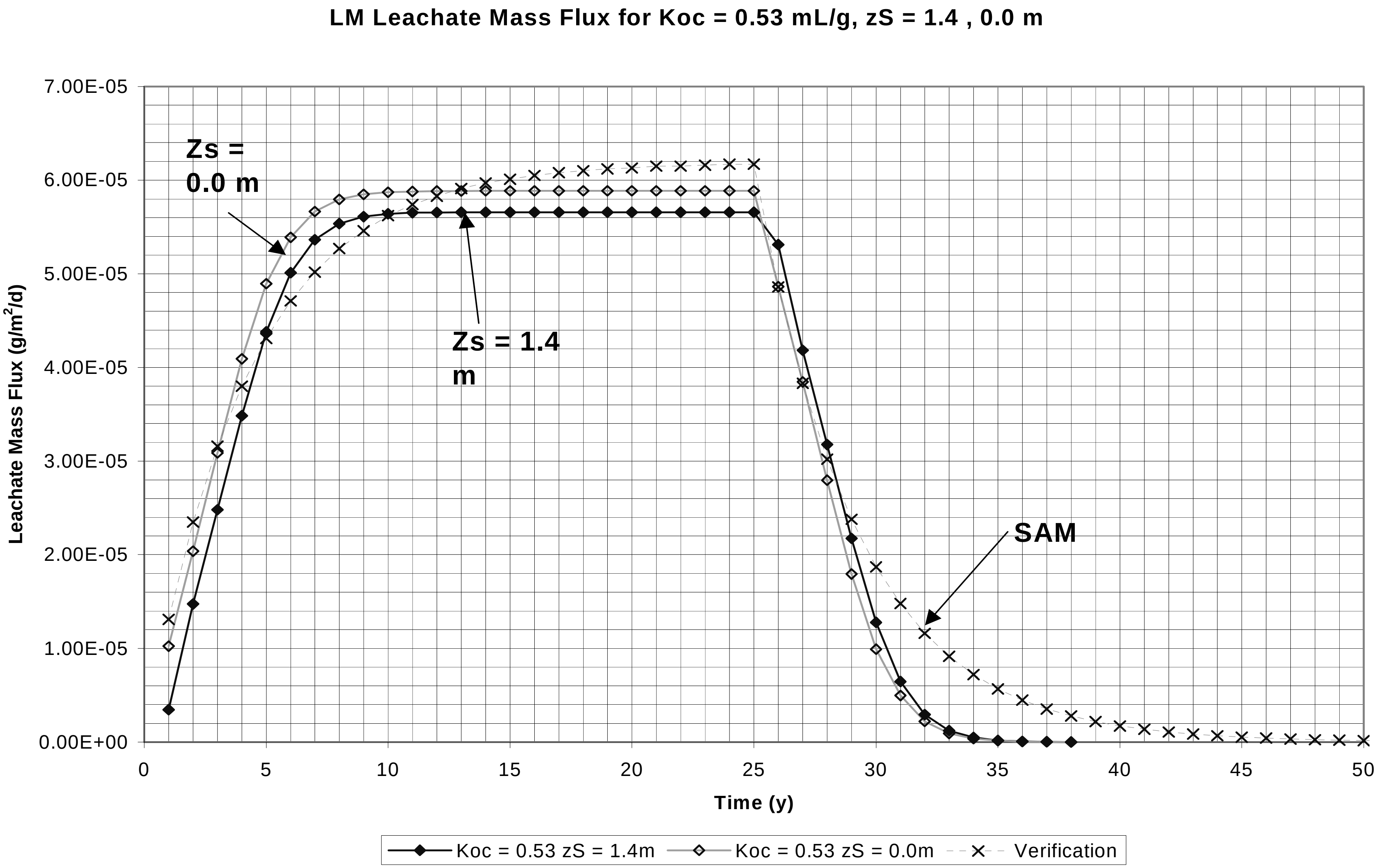

Figure 1a Comparison of Leachate Mass Fluxes Generated by the HWIR99 Landfill Module with Zs = 0.0 and 1.4 m, and the Semi-Analytical Model (SAM), K_{oc} = 0.53 mL/g.

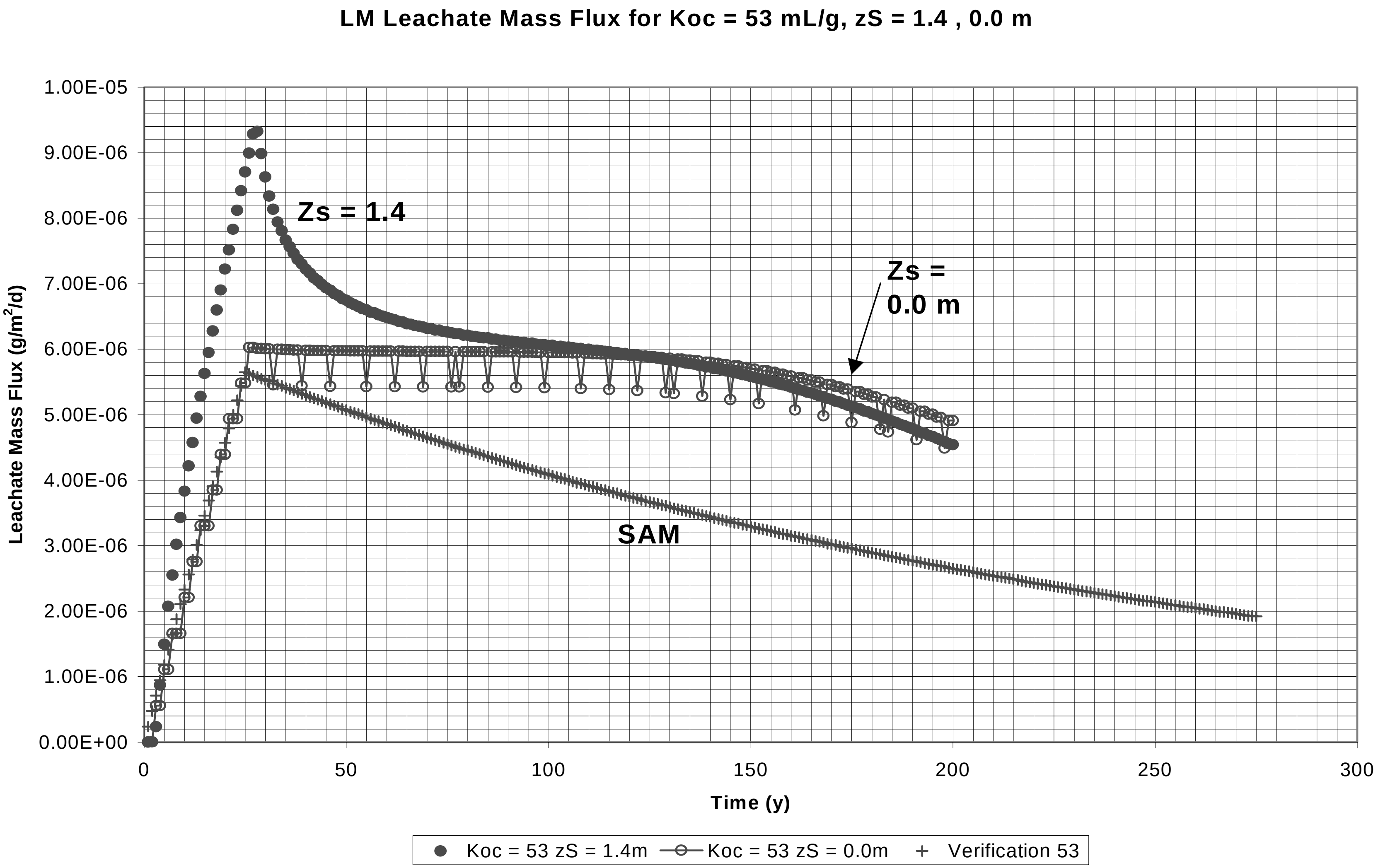

Figure 1b Comparison of Leachate Mass Fluxes Generated by the HWIR99 Landfill Module with Zs = 0.0 and 1.4 m, and the Semi-Analytical Model (SAM), K_{oc} = 53 mL/g.

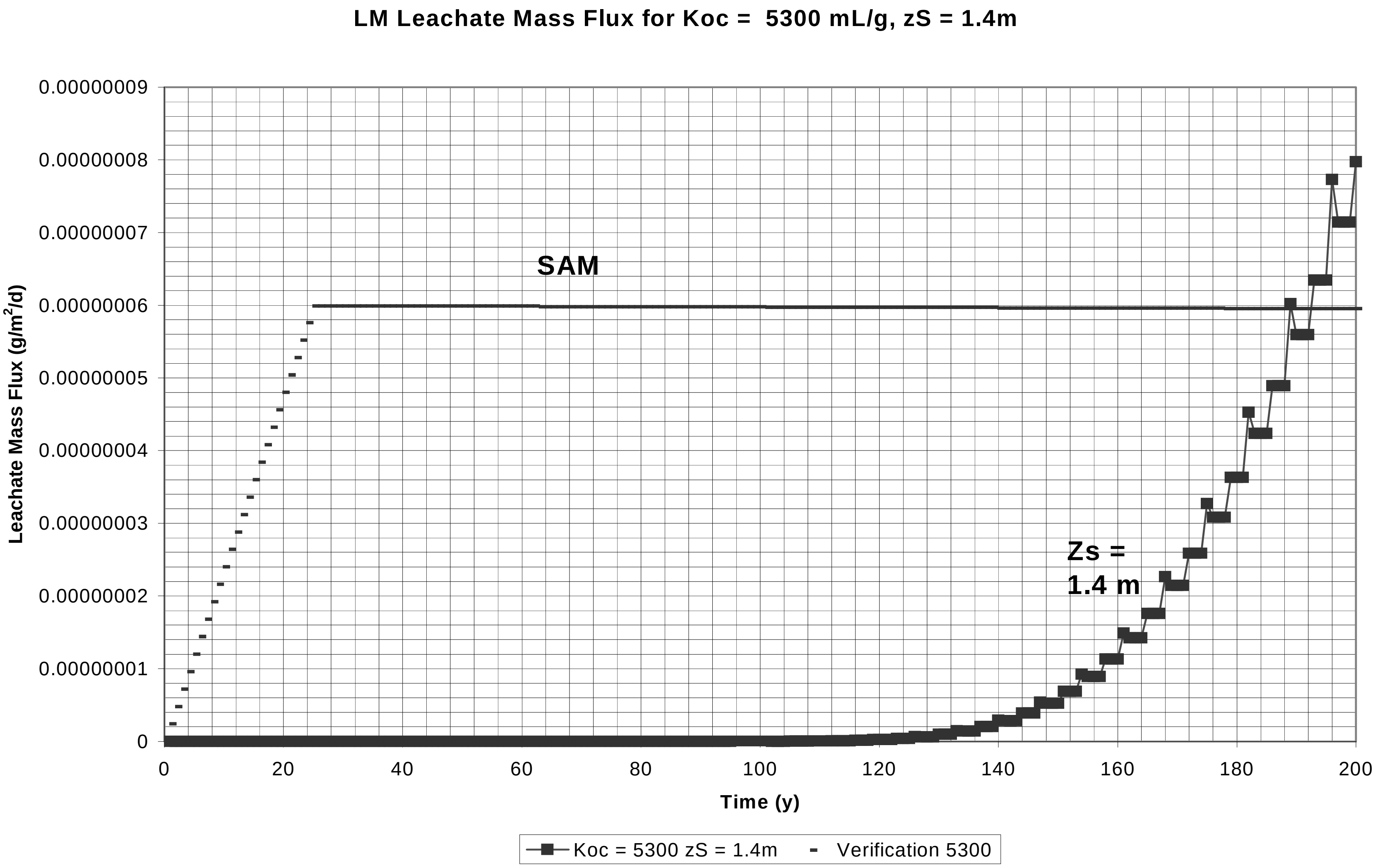

Figure 1c **Comparison of Leachate Mass Fluxes Generated by the HWIR99 Landfill Module with Zs = 0.0 and 1.4 m, and the Semi-Analytical Model (SAM), K_{oc} = 5,300 mL/g.**

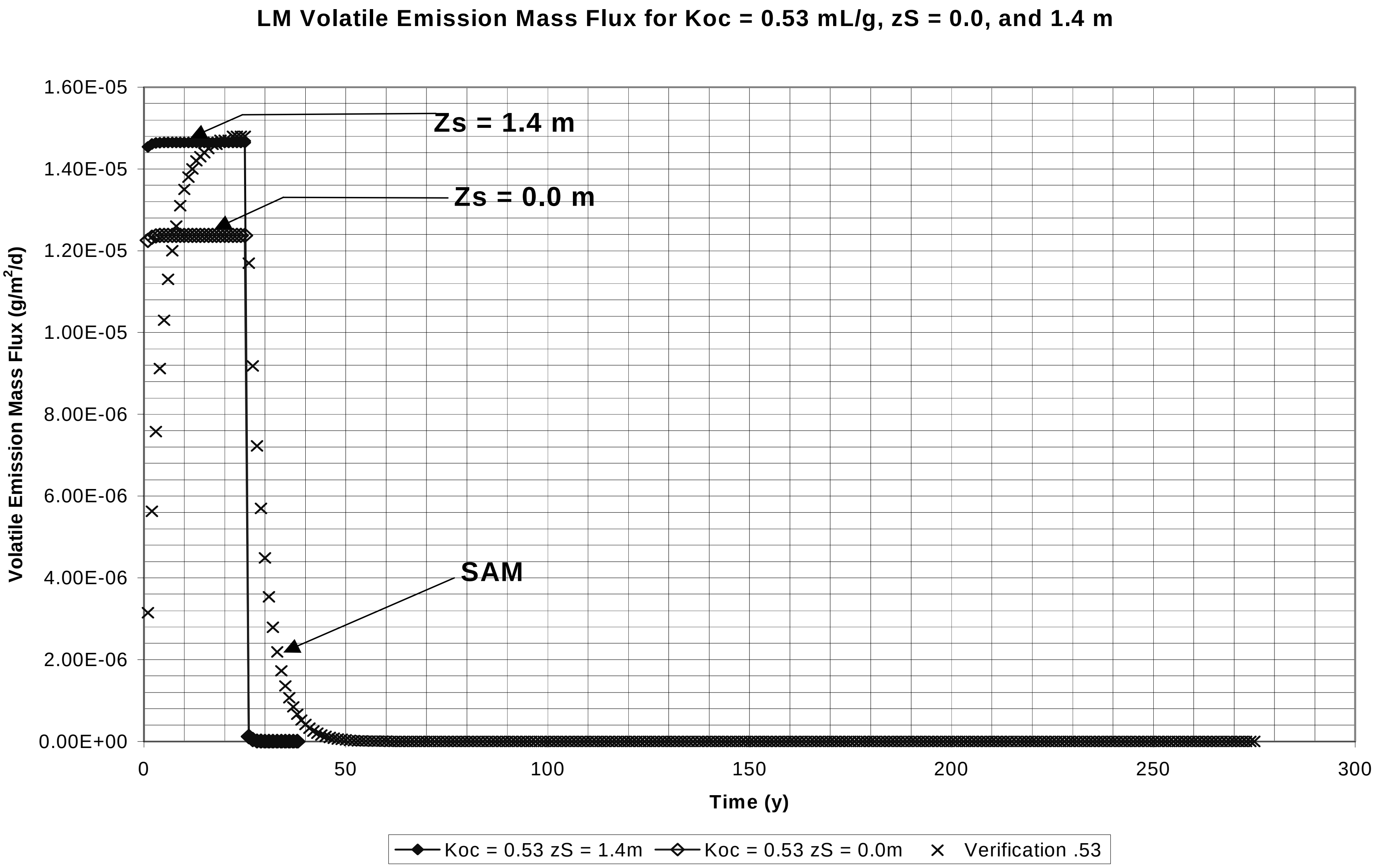

Figure 2a Comparison of Volatile Emission Mass Fluxes Generated by the HWIR99 Landfill Module with Zs = 0.0 and 1.4 m, and the Semi-Analytical Model (SAM), K_{oc} = 0.53 mL/g.

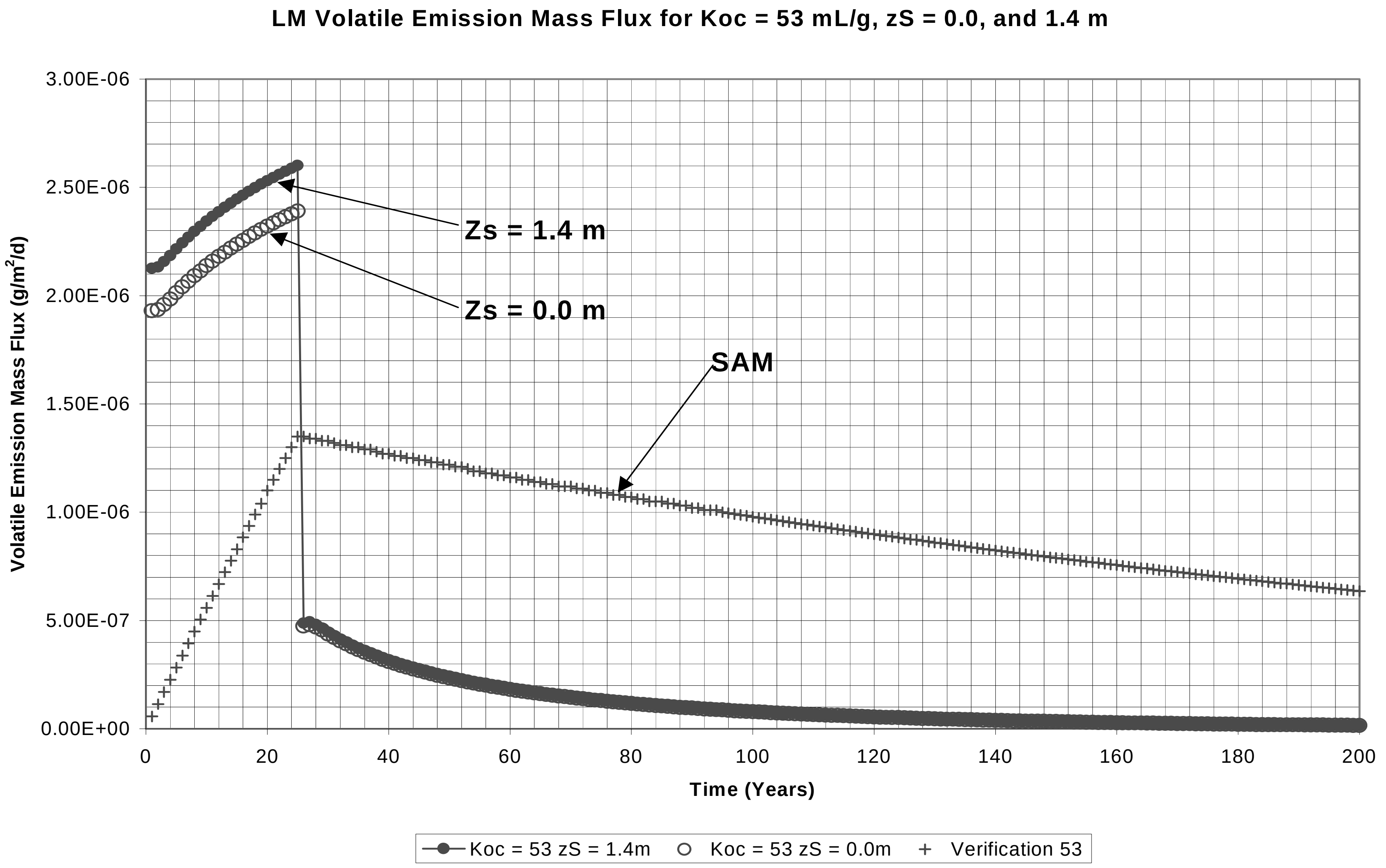

Figure 2b Comparison of Volatile Emission Mass Fluxes Generated by the HWIR99 Landfill Module with Zs = 0.0 and 1.4 m, and the Semi-Analytical Model (SAM), K_{oc} = 53 mL/g.

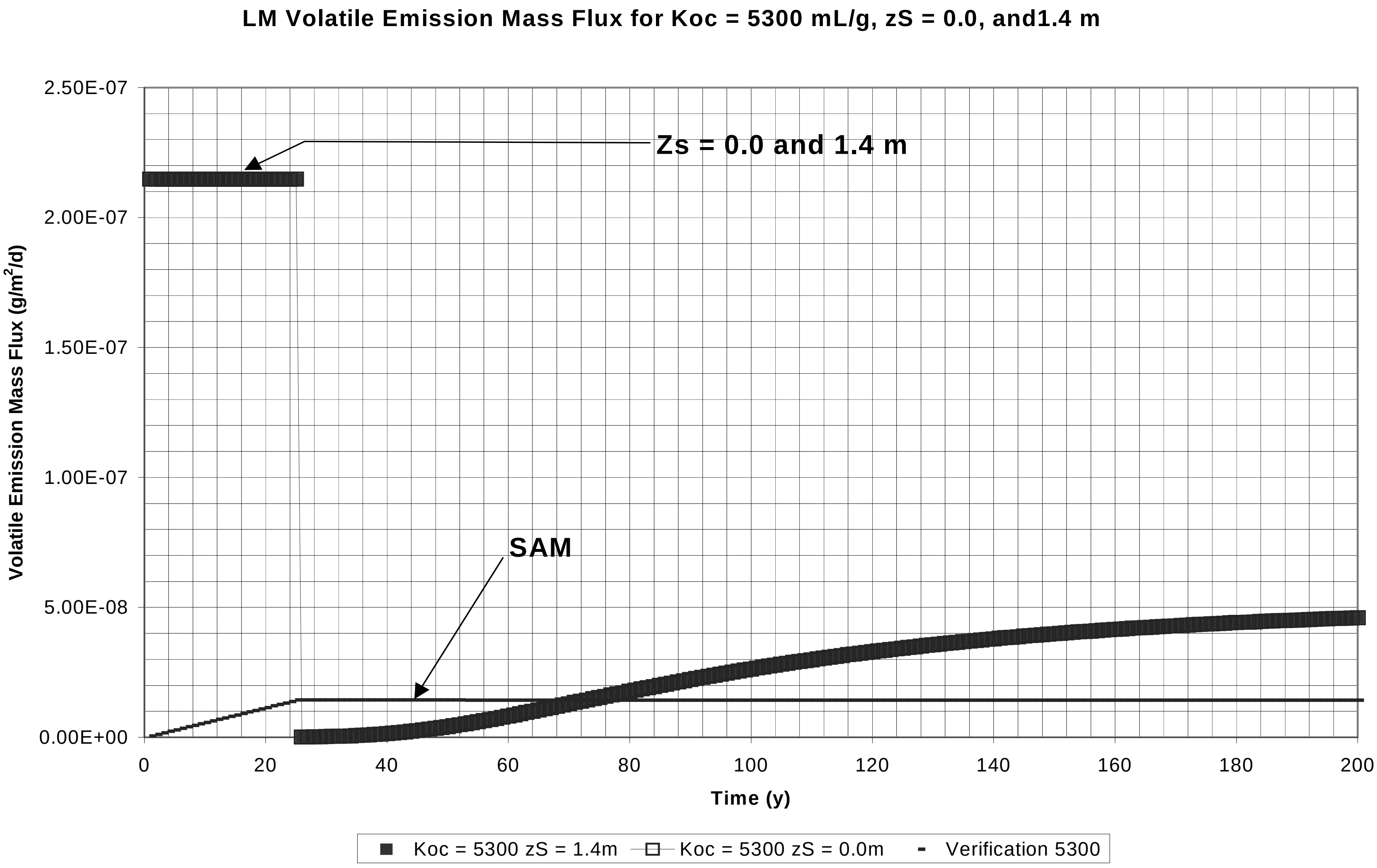

Figure 2c **Comparison of Volatile Emission Mass Fluxes Generated by the HWIR99 Landfill Module with Zs = 0.0 and 1.4 m, and the Semi-Analytical Model (SAM), K_{oc} = 5,300 mL/g.**

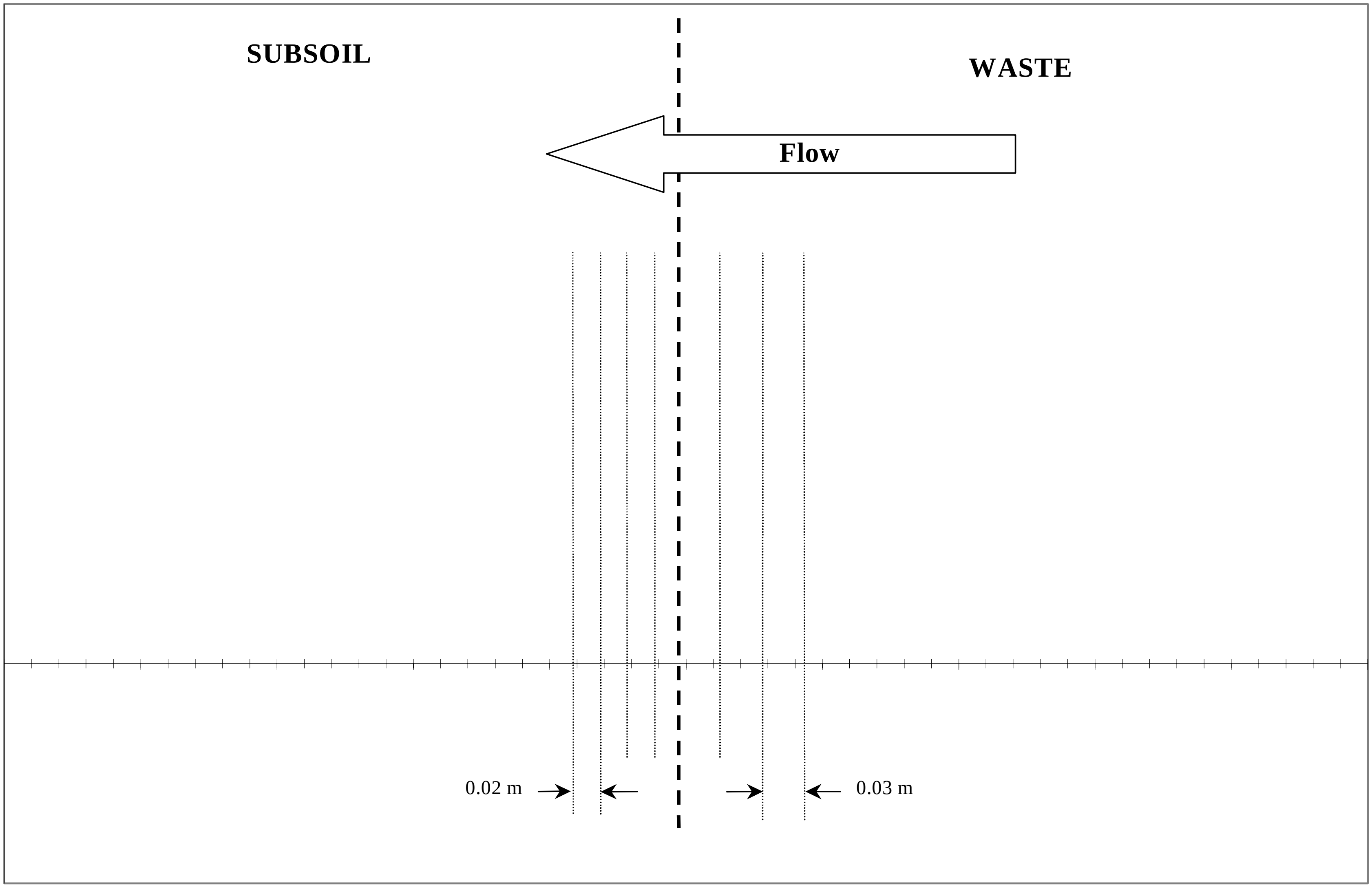

Figure 3 Discretizations in the Subsoil and Waste Zones near the Interface between the two Materials.

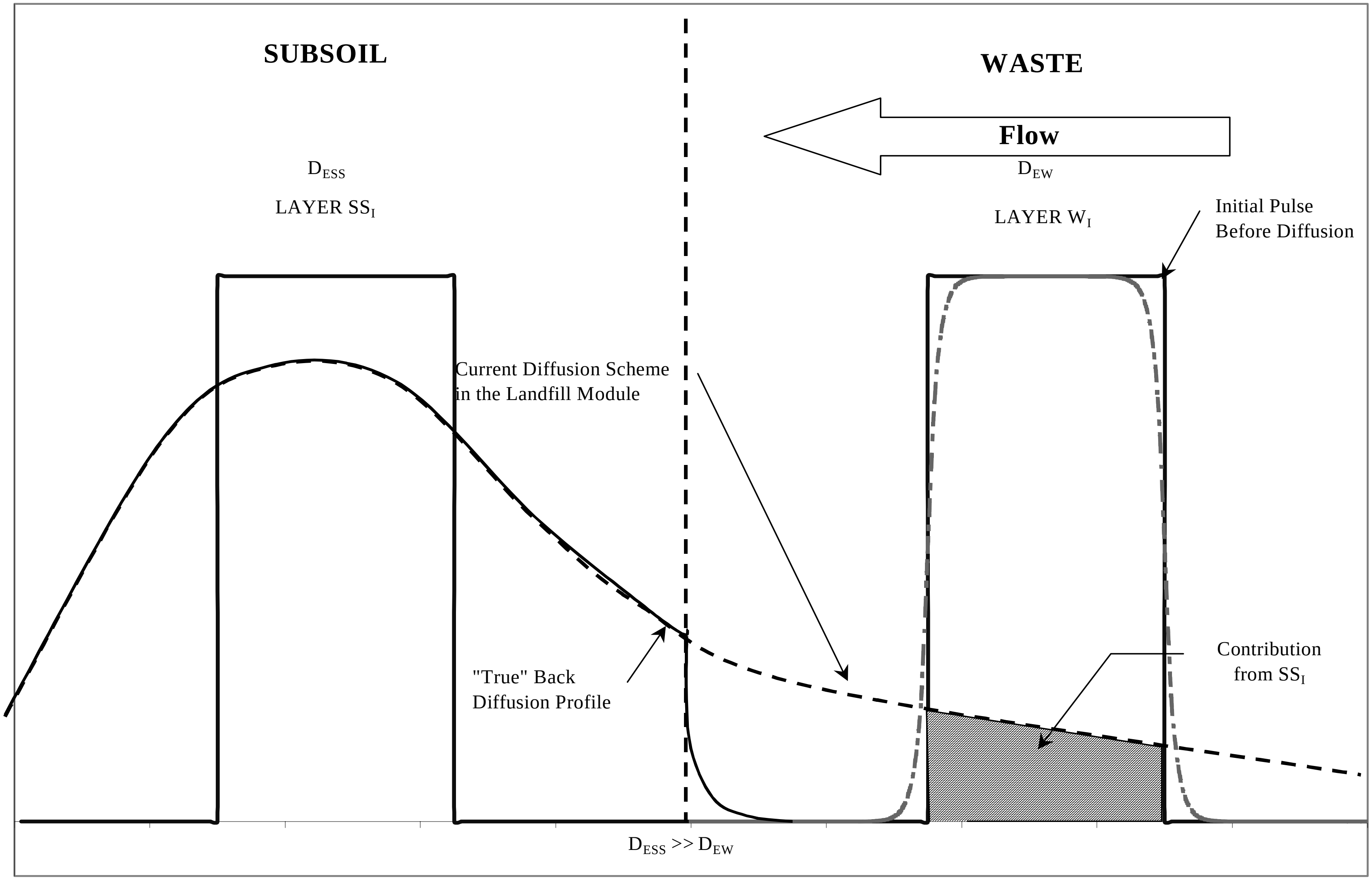

Figure 4 **A Schematic Showing Diffusion in the Subsoil and Waste Zones.**

APPENDIX A

CALCULATION OF MAXIMUM LEACHATE CONCENTRATION AND FLUX

The maximum leachate concentration cannot exceed aqueous concentration at equilibrium, viz:

$$C_T = \rho_{HW} C_W f_{WMU} = K_{TL} C_L \tag{A.1}$$

The maximum leachate concentration must obey the following limit:

$$C_{Lmax} \leq \frac{\rho_{HW} C_W f_{WMU}}{K_{TL}} \tag{A.2}$$

The maximum leachate flux may be approximated by:

$$F_{\max} = I C_{Lmax} \tag{A.3}$$

where:

$$K_{TL} = \rho_b f_{oc} K_{oc} + \theta S_w + \theta S_a H' \tag{A.4}$$

C_L = Leachate concentration (kg/m^3)
C_{Lmax} = Maximum leachate concentration (kg/m^3)
C_W = Waste concentration (kg/kg) = 1 x 10^{-6}
ρ_{HW} = Waste dry density (kg/m^3) = 1395
ρ_{Liner} = Liner dry density (kg/m^3) = 1458
V = Disposed waste volume (m^3) = 8,944
V_{cp} = Landfill capacity (m^3) = 8,944
A = Area of landfill (m^2) = 2,023.5
θ = Porosity of the waste column = 0.63
θ = Porosity of the landfill cover = 0.45
S_w = Degree of saturation of water of the waste column = 0.794
S_{wliner} = Degree of saturation of water of the liner = 0.608
S_a = Degree of saturation of air = 0.206
f_{oc} = Organic carbon fraction = 0.848
f_{WMU} = Waste fraction = 0.103
K_{oc} = Equilibrium partitioning coefficient normalized to organic carbon (m^3/ kg) = 0.053

I = Infiltration rate (m/a) = 0.956
H' = Henry's constant (unitless) = 0.141 = 0.003273 (atm m^3/ mol)

Using Equation (A.4):

for the waste column, K_{TL} = 63.2 (unitless), and
for the liner, K_{TL} = 2 (unitless).

Using Equation (A.2),

$$C_{Lmax} = 1395 \times 1 \times 10^{-6} \times 0.103/ 63.2 = 2.27 \times 10^{-6}\ kg/m^3$$

Maximum leachate flux is therefore:

$$Flux = 0.956 \times 2.27 \times 10^{-6} \times 1000/ 365 = 5.95 \times 10^{-6}\ g/ m^2/ d$$

APPENDIX B

COMMENTS ON THE ADDITIONAL CHANGES TO THE LANDFILL MODULE.

B.1 BACKGROUND

After the completion of the verification document, HydroGeoLogic has received another technical memorandum with additional results from RTI (RTI, 1999, attached at the end of this Appendix). In the memorandum, results from the following two runs were reported.

- Liner thickness = 0.0 m, Landfill cover thickness = 0.0 m; and
- Liner thickness = 0.0 m, Landfill cover thickness = 1.4 m.

An analytical solution is available for the scenario with no landfill cover. A brief description of the solution is shown below.

With the governing transport equation:

$$\begin{gathered}(\theta S_w + (1-\theta)K_d\rho_s + \theta H'S_a)\frac{\partial C}{\partial t} + I\frac{\partial C}{\partial z} = \frac{\partial}{\partial z}(\theta S_w D_{wEff} + \theta H'S_a D_{aEff})\frac{\partial C}{\partial z} \\ -\lambda(\theta S_w + (1-\theta)K_d\rho_s)C \\ z \quad \in \quad (0, z_L)\end{gathered} \tag{B.1}$$

and the following initial and boundary conditions:

a) Initial Condition

$$C(z,o) \quad = \quad C_0, for \;\; all \;\; z \tag{B.2}$$

b) Condition at the Bottom Boundary

$$\frac{\partial C}{\partial z} \quad = \quad 0, at \;\; z \; = \; z_L \tag{B.3}$$

c) Condition at the Top Boundary

$$C \quad = \quad 0, \;\; at \;\; z \; = \; 0 \tag{B.4}$$

where

t = Time

C = Leachate concentration

I = Infiltration rate

H' = Henry's constant

θ = Porosity of the waste

S_w = Water saturation of the waste

S_a = Air saturation of the waste

D_{aEff} = Effective diffusion coefficient for benzene in air

$$= \frac{(\theta S_a)^{\frac{7}{3}} D_a}{\theta^2}$$

D_a = Molecular benzene diffusivity in air.

D_{wEff} = Effective diffusion coefficient for benzene in water

$$= \frac{(\theta S_w)^{\frac{7}{3}} D_w}{\theta^2}$$

D_w = Molecular benzene diffusivity in water.

z = Vertical distance from the top of the waste column

z_L = Vertical distance from the top of the waste column to the bottom the waste column, i.e., waste column thickness.

Equation (B.1) along with Conditions (B.2), (B.3), and (B.4), may be solved by Laplace transformation to give the following general solution:

$$\overline{C}(z,p) = A_1 \exp(r_1 z) + A_2 \exp(r_2 z) + \frac{\alpha C_0}{\alpha p + \lambda\gamma} \tag{B.5}$$

where

$$\alpha = \gamma + \theta S_a H'$$

$$\beta = \theta S_w D_{wEff} + \theta S_a H' D_{aEff}$$

$$\gamma = \theta S_w + (1-\theta) K_d \rho_s$$

$$r_i = r_i(z_L,\ \alpha,\ \beta,\ \gamma,\ I,\ p)$$

$$A_i = A_i(z_L,\ \alpha,\ \beta,\ \gamma,\ I,\ p)$$

p = Laplace transform parameter
$\overline{C}$ = Transformed concentration in Laplace space
r_i = root i of the Laplace-transformed transport equation.
A_i = Constant i in Equation (B.5)

$\overline{C}$ is transformed numerically using the deHoog's method (deHoog, 1982).

B.1.1 Comparison of Leachate Fluxes at the Bottom of the Waste Column

Leachate fluxes at the bottom of the waste column versus time for a single landfill cell associated with the LM, and the analytical solution described above are shown in Figure B.1. The analytical solution predicts almost constant leachate fluxes during the first 150 years of emplacement. After 150 years, the leachate fluxes gradually decrease. A similar behavior of LM is also observed in Figure B.1. However, the LM flux during the 200-year LM simulation period is consistently 10 percent smaller than those predicted by the analytical solution. Values of annual leachate fluxes predicted by LM and the analytical solution during the first 35 years of simulation are presented in Table B.1.

The values of leachate flux at the bottom of the waste column predicted by the analytical solution during the first 150 years of simulation are equal to the product of the initial aqueous concentration at equilibrium and the infiltration rate, I C. The calculation is shown below.

$$\text{Leachate flux (g/m}^2\text{/d)} = IC = I\left(f_{WMU}\frac{C_w}{K_{TL}}\rho_{HW}\right)$$

$$= 0.956/365 \text{ (m/d) x [} 0.103 \text{ x } 0.1 \text{ (g/g)}/63.2 \text{ x } 1395 \text{ x } 1000 \text{ g/m}^3 \text{]}$$

$$= 0.595 \text{ g/m}^2\text{/d}$$

B.1.2 Comparison of Volatile Emission Fluxes at the Top of the Waste Column

Volatile emission fluxes at the top of the waste column versus time for a single landfill cell associated with the LM, and the analytical solution described above are shown in Figure B.2. Both the LM and the analytical solution show similar characteristics, both decreasing with time. However, oscillation in the LM solution is observed. In addition, it is noted also that the volatile emission flux predicted by LM is consistently greater than that by the analytical solution. As can be seen in Figure B.2, the difference increases with time. The difference between the LM and analytical solution may be as great as two orders of magnitude at 200 years. Values of annual volatile emission fluxes predicted by LM and the analytical solution during the first 35 years of simulation are presented in Table B.1.

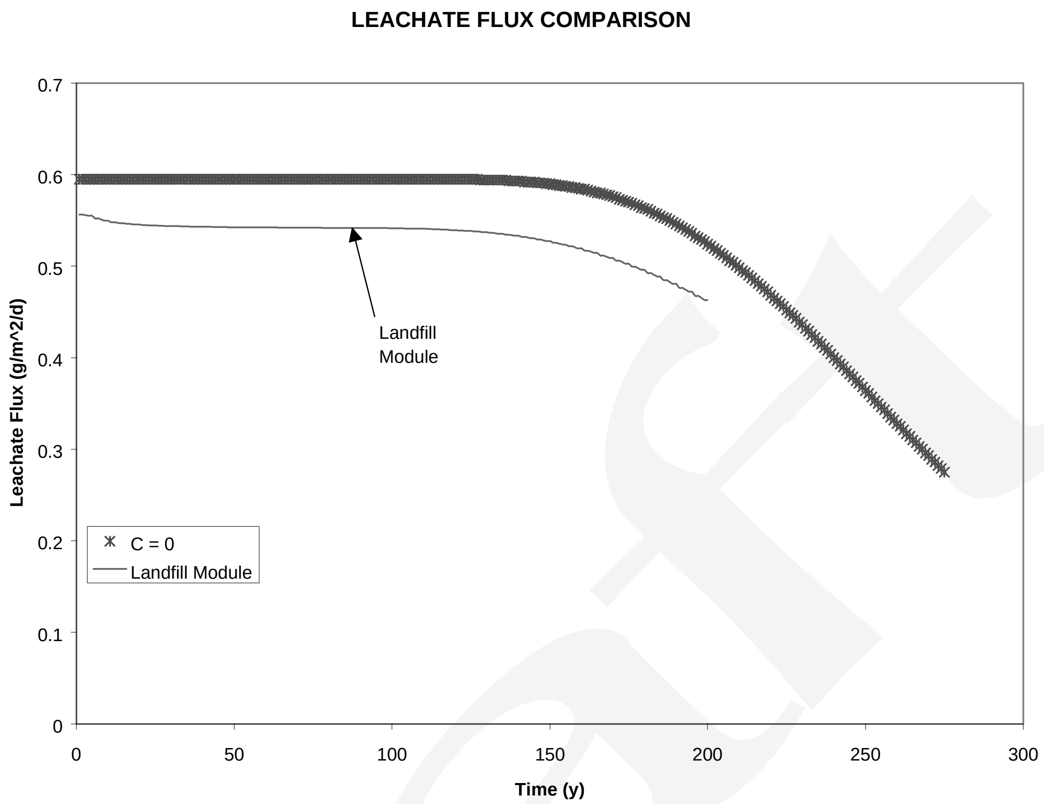

Figure B.1 **Comparison between LM and the Analytical Solution: Leachate Flux Versus Time**

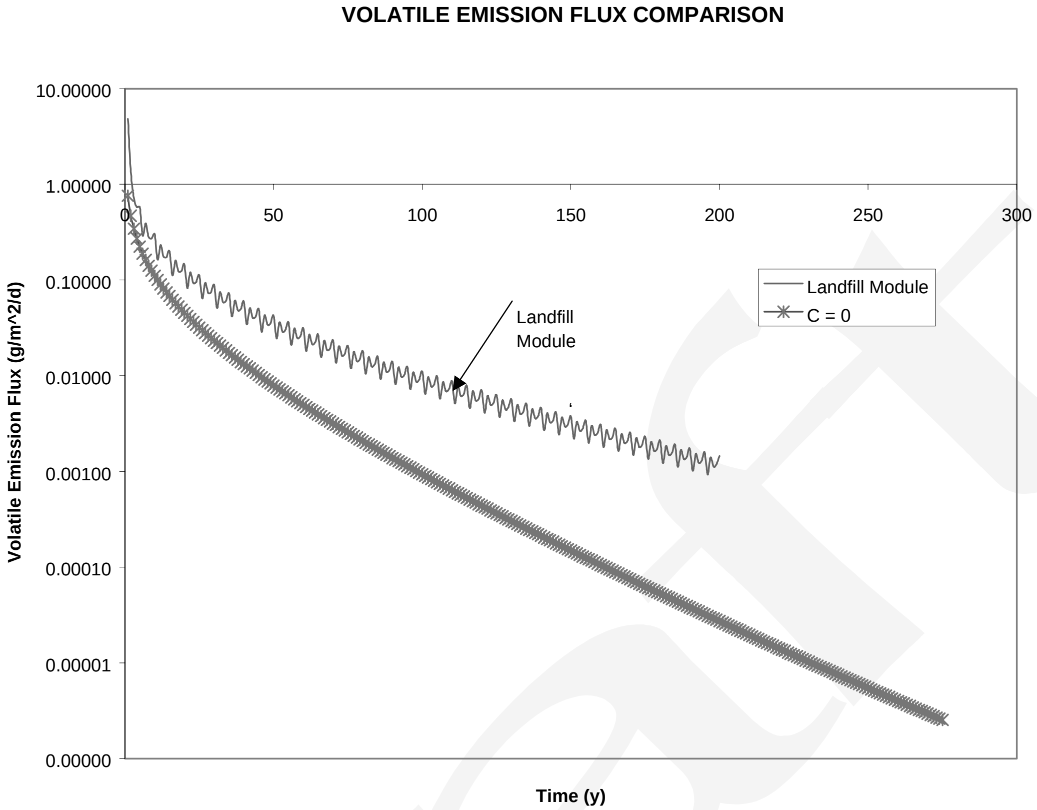

Figure B.2 Comparison between LM and the Analytical Solution: Volatile Emission Flux Versus Time

Table B. 1 Comparison of Leachate and Volatile Emission Fluxes for the First 35 Years

	Leachate Flux g/m^2/d		Volatile Emission Flux g/m^2/d	
YEAR	LM	Analytical Solution	LM	Analytical Solution
1	0.55643	0.595	4.83496	0.76
2	0.55643	0.595	1.36128	0.469
3	0.55563	0.595	0.72099	0.344
4	0.55484	0.595	0.57718	0.271
5	0.55484	0.595	0.57878	0.223
6	0.55205	0.595	0.29086	0.188
7	0.55205	0.595	0.38984	0.162
8	0.55087	0.595	0.28257	0.141
9	0.54969	0.595	0.26992	0.125
10	0.54969	0.595	0.30235	0.111
11	0.54802	0.595	0.16389	0.0997
12	0.54802	0.595	0.23147	0.0899
13	0.54743	0.595	0.17505	0.0815
14	0.54685	0.595	0.17356	0.0743
15	0.54685	0.595	0.20050	0.0679
16	0.54601	0.595	0.11146	0.0623
17	0.54601	0.595	0.16061	0.0573
18	0.54569	0.595	0.12363	0.0529
19	0.54537	0.595	0.12466	0.049
20	0.54537	0.595	0.14618	0.0454
21	0.54486	0.595	0.08232	0.0422
22	0.54486	0.595	0.11990	0.0392
23	0.54466	0.595	0.09321	0.0366
24	0.54445	0.595	0.09490	0.0342
25	0.54445	0.595	0.11227	0.0319
26	0.54411	0.595	0.06372	0.0299
27	0.54411	0.595	0.09344	0.028
28	0.54397	0.595	0.07310	0.0263
29	0.54382	0.595	0.07489	0.0247
30	0.54382	0.595	0.08914	0.0233
31	0.54358	0.595	0.05086	0.0219
32	0.54358	0.595	0.07493	0.0206
33	0.54347	0.595	0.05887	0.0195
34	0.54337	0.595	0.06059	0.0184
35	0.54337	0.595	0.07243	0.0173

B.2 TECHNICAL MEMORANDUM FROM RTI

Memorandum

To: Zubair Saleem, EPA, Stephen Kroner, EPA, Dua Guvanasen, HGL
cc: Keith Little, RTI, Terry Pierson, RTI
From: Paula Labieniec, RTI
Date: June 4, 1999
Subj: Interim Recommendations on Landfill Module

In light of the recent discussions regarding the appropriate inner boundary conditions (cover soil/waste and waste/subsoil) for use in the landfill module and the tight time constraints, we make the following interim recommendations. Even though subsoil zone is zeroed out in the current production runs, we are including this zone in our recommendations to be complete.

Cover Soil/Waste Boundary

At this boundary, we agree with the review comments from HydroGeologic that a boundary condition should be applied where the sum of the advective and diffusive fluxes on either side of the boundary are equal. However, using the current solution technique, we have no means of implementing such a rigorous boundary condition in the time allowed. As an environmentally conservative alternative that is easily implemented with slight modification to the current code, we recommend the following:

- at the bottom of the cover soil zone, applying a no diffusive flux (dCT/dz=0) boundary condition where CT is the total contaminant concentration.
- at the top of the waste zone, applying a CT=0 boundary condition to determine the diffusive flux from the waste zone into the cover soil.

This allows advective transfer, but not diffusive transfer, of contaminant mass from the cover soil to the waste zone. Use of these conditions would tend to over-estimate contaminant mass losses from the waste zone into the cover soil zone and over estimate the volatile flux. This would address HydroGeologic's comment that in the current version, we are over estimating back-diffusion from cover soil to waste and thus, *under*estimating volatile emissions when a cover is in place.

These boundary conditions were implemented in a test version of the code. Figure 1 provides a comparison of the results using the version of the landfill module in the current HWIR ('Cur' in the Figure 1 key) executable and the modified test version ('Mod' in the Figure 1 Key) with a cover soil zone of 1.4m. The input files for LF0223504 (with zS=0) and for benzene were used. These are the same input files used by HydroGeologic in their analyses (5/6/99 and 5/26/99). Results for the case where zS=0 and zC=0 are the same in both versions of the model and are provided here for comparison.

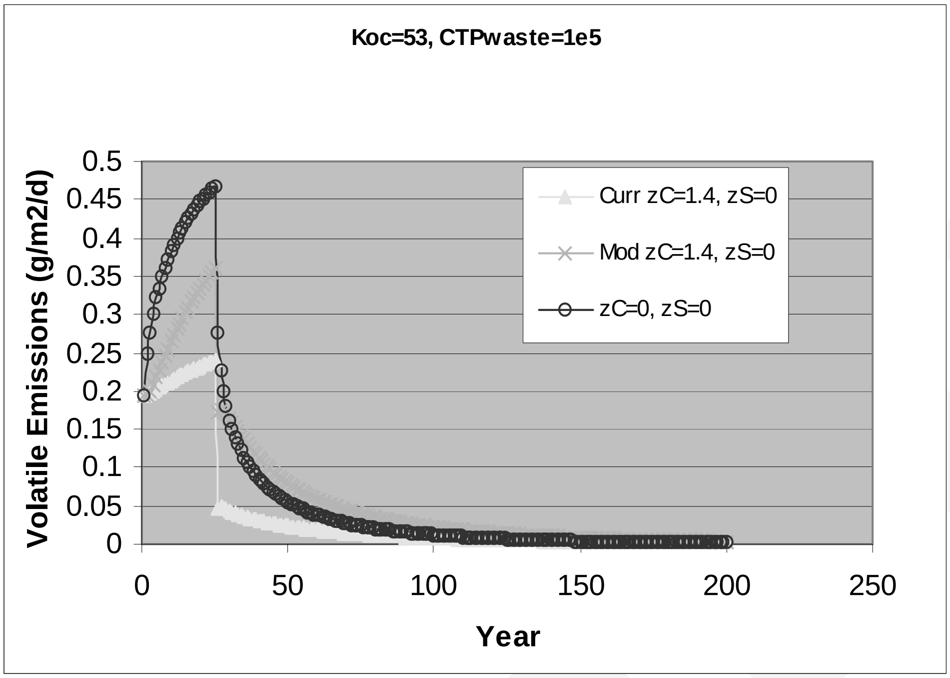

Figure 11 Volatile Emissions over Time

Waste/Subsoil Boundary
At this boundary, HGL has recommended a boundary condition where dCL/dz=0 . CL is the aqueous phase contaminant concentration in the soil pore water. Since diffusive flux occurs in the aqueous and gas phases only, dCL/dz=0 implies no diffusive flux across this boundary, this boundary condition can be approximated by:

- at the bottom of the waste zone, setting the boundary condition equal to dCT/dz=0 which prevents diffusive flux from waste to subsoil
- modeling only advection and decay only in the subsoil zone. Since no diffusion is modeled, there will be no diffusive transfers from subsoil to waste.

As for Figure 1, leach flux results were generated using the version of the landfill module in the current HWIR ('Cur' in the Figure 2 key) executable and the modified test version ('Mod' in the Figure 2 Key) which implements these boundary conditions. The input files for LF0223504 and for benzene were used . These are the same input files used by HydroGeologic in their analyses (5/6/99 and 5/26/99). Figure 2a illustrates the differences in leach flux versus time profiles when a suboil zone of 1.4m (zS=1.4m) is simulated. In addition, the leach flux over time when there is no subsoil (and zC=1.4) is illustrated. Results for the case where zS=0 are approximately the same in both versions of the model and are provided here for comparison. Figure 2b shows the leach flux for the first 30 years to highlight the fact that, with the modifed version of the model, the existence of a subsoil zone simply shifts the leach flux profile by 3 years, the amount of time required for the contaminant to travel from the top to the bottom of the subsoil zone calculated using:

SSTime=zS*KTLs/I/365

where.

zS = thickness of subsoil, m = 1.4

I = infiltration rate,m/d = 0.0026

KTLs = the total/aqueous phase partition coefficient in the subsoil =2.1 (see eq.2.1-7 in documentation.)

In addition, the theoretical maximum leach flux rate (0.6 g/m2/d) can be calculated using:
Fmax= I*BDw*Cw*fwmu/KTLw

where:

BDw = the waste dry bulk density, g/cm3 = 1.395

Cw = contaminant concentration in waste, dry basis,μg/g = 1e5

fwmu = fraction hazardous waste = 0.105

KTLw = the total/aqueous phase partition coefficient in the waste = 63.6 (see eq.2.1-7 in documentation.)

Figures 2a and 2b show that this calculated theoretical maximum leach flux is not exceeded the modified version of the model whereas it is in the current version.

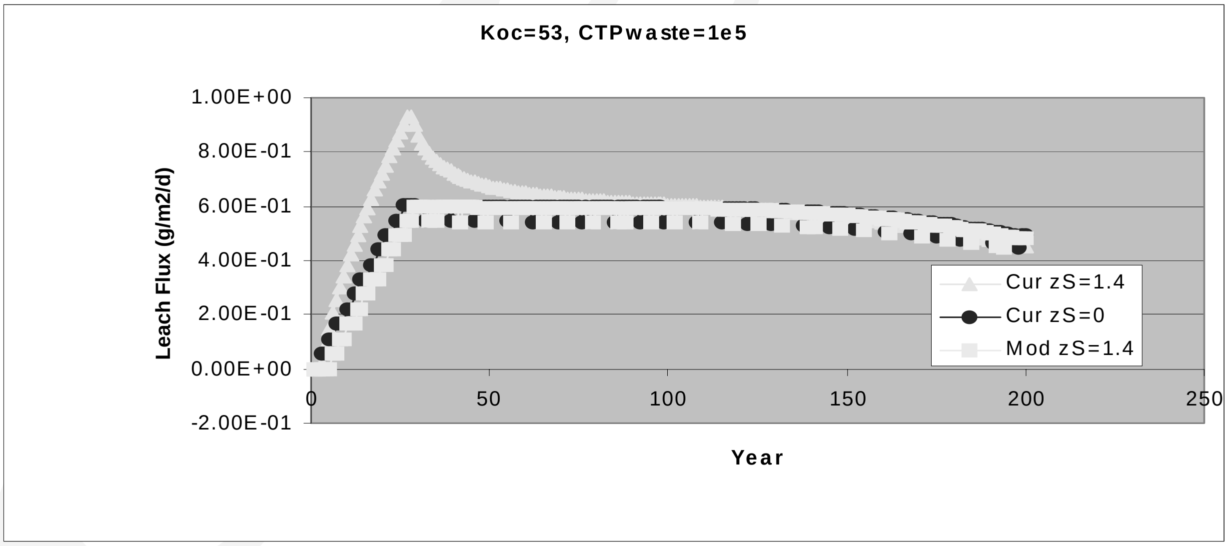

Figure 12a: Leach Flux over time

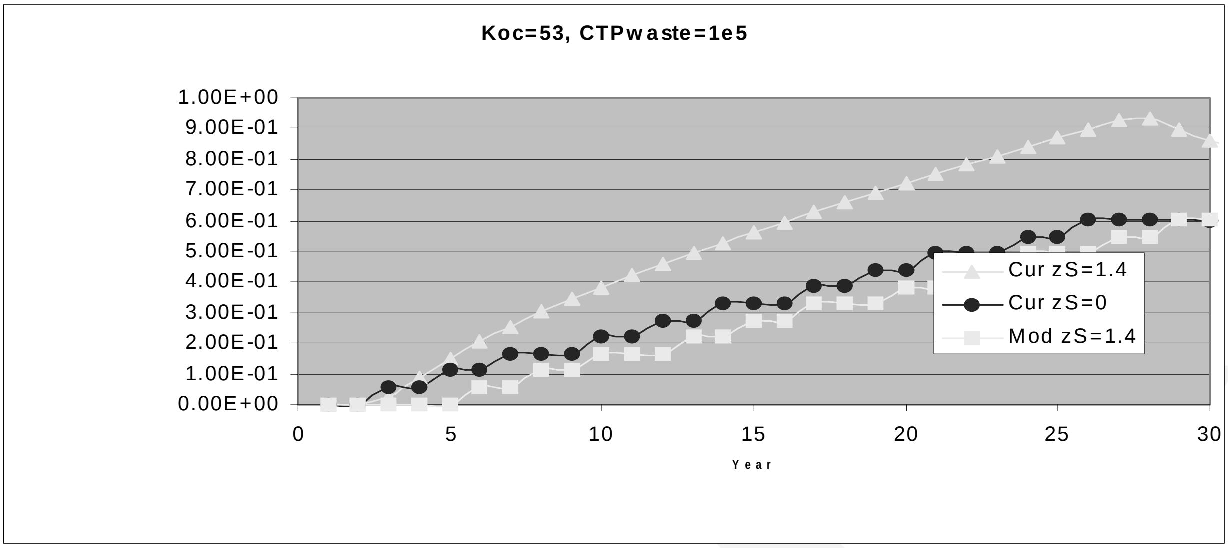

Figure 2a: **Leach Flux profile, first 30 years**

Appendix C

Verification of Particulate Emission

The landfill module provides an estimate of the annual average emission rate of contaminant mass adsorbed to particulate matter. The module accounts for four release mechanisms: wind erosion, vehicular activity, spreading/tilling/compaction, and unloading. The module was verified by performing hand calculations with the equations presented in the Source Models for Non-Wastewater Waste Management Units (Land Application Units, Waste Piles, and Landfills). The parameter values used in the hand calculations is shown below in Table C1

Table C1. Input Variables and Values for Landfill Particulate Emission Calculations.

Parameter Description	Variable	Value	Unit
Silt Content of roadway	**S**	25.988	w/w %
Mean Vehicle Speed	**vs**	33.94	km/h
Mean Vehicle Weight	**vw**	22.5	Mg
Mean Number of Vehicles Per Day	**nv**	0.0894	1/day
Mean Number of Wheels Per Vehicle	**nw**	6	--
Dust Suppression Control Efficiency	**effdust**	0.1971	--
Meters Traveled	**mt**	44.983	m
Source Area	**area**	2023.5	m^2
Mean Number of Days Per Year With > = 0.01 Inches of Percipitation	**P**	139	day
Number of Tilling/Spreading/Comaction Actions Per Day	**Nopp**	0.44708	1/day
Mean Annual Wind Speed	**u**	4.349	m/s
Moisture Content of Waste	**mcW**	50	%
Annual Average Waste Loading Rate	**load**	489.98	Mg/year
Number of Waste Cells in Landfill	**ncell**	25	--

The particulate emission for each release mechanism is calculated separately and then summed to determine total particulate emissions. The calculations are based on the assumption that the entire landfill area is contributing to the particulate emission. The module, however, only allows mass contributions from the active landfill cell. Therefor, the total particulate emission mass flux rate is divided by the number of landfill cells.

Wind erosion (E30wd)

E30wd not calculate(=0.0) because average wind velocity below threshold.

Vehicular activity

$$E30_{ve} = 1.36 * \left(\frac{S}{12}\right) * \left(\frac{vs}{48}\right) * \left(\frac{vw}{2.7}\right)^{0.7} * \left(\frac{nw}{4}\right)^{0.5} * \frac{(365-P)}{365} * nv * (1-effdust) * \left(\frac{mt}{area}\right)$$

$E30_{ve}$ = 0.011116796.

Spreading/Tilling/Compaction

$$E30_{sc} = 1.77 * S^{0.6} * Nopp * 0.1$$

$E30_{sc}$ = 0.558756031.

Unloading

$$E30_{un} = 0.012 * \frac{\left(\frac{u}{2.2}\right)^{1.3}}{\left(\frac{ncW}{2}\right)^{1.4}} * \frac{load}{area} * \frac{1000}{365}$$

$E30_{un}$ = 2.1311E-05.

The sum of $E30_i$/ncells = 0.569894138 / 25 = 0.022795766. This value matches what the landfill module predicted for the verification case.