Contamination transport into saturated land upon advection-diffusion-sorption including decay

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Abstract:

The objective of this paper is to describe governing numerical equation and solution algorithm of pollution transport mechanisms and factors essential to include in developing relatively simple and practical tools to quantify pollution loss, advection, diffusion and sorption in pollution transport into the groundwater at landfill sites.

This paper presents the development of a numerical model that can be used for quantifying groundwater inputs and associated contaminant discharge from a landfill into the affected aquifer. The results reveal that the proposed model can be used for the simulation of contaminant transport in aquifers in any scale. This numerical solution is established on finite difference-finite volume solution advection-diffusion-linear sorption with first order decay equation. To show the capability of proposed model, the results of a case study presented in the paper as simulating leachate transport at a 2000 ton/day landfill facility assesses leachate migration away from the landfill in order to control associated environmental impacts, particularly on groundwater wells down gradient of the site. Leachate discharge from landfills is the main route for release of the organic and inorganic contaminants through subsurface, commonly encountered in the refuse. Leachate quantity and potential percolation into the subsurface are estimated by the proposed model. A comprehensive sensitivity analysis to leachate transport control parameters was also conducted. Sensitivity analysis suggest that changes in source strength, aquifer hydraulic conductivity, and dispersivity have the most significant impact on model output indicating that these parameters should be carefully selected when similar modeling studies are performed. The sensitivity of the model to variations in input parameters results in two opposing patterns of contaminant concentration. While higher groundwater velocities increase the speed of plume spread, they also increase the dilution ratio and hence Decrease the concentration.

1. Introduction

To predict the fate of contaminant transport through groundwater, an accurate numerical modeling is required. Several approaches have been developed to improve the numerical accuracy. Among the numerical methods for solving ADRE, finite difference method (FDM) and finite volume method (FVM), seems to be more popular for the ease of implementation and their relative simplicity (Ataie et al., 1999[1]; Moldrup et al., 1996[2]; Stanbro et al., 2000[3]; Shue et al., 2000[4]). However, finite element method (FEM) can easier handle complex geometries. There have been extensive debates as to whether FEM or FDM is preferable in groundwater modeling (Zheng et al.,

1990[5]. Some investigation showed that FDM introduces larger numerical errors than FEM (Noye et al., 1990[6]; Hossain et al., 1999[7]; Liu et al., 1996[8]; Sheu et al., 2002[9]) and discussed in many standard books on the subject (e.g. Zheng and Bennett, 2002[10]. (Albaiges et al., 1986[11]; Dunlap et al., 1976[12]; El-Fadel et al., 1997a[13]; Garland and Mosher, 1975[14]; MacFarlane et al., 1983[15]; Malina et al., 1999[16]; Reinhard et al., 1984[17]; Zanoni, 1972[18]). This created the need to understand the mechanisms that control leachate formation, quality, quantity, and most importantly migration characteristics with associated spatial and temporal variations during landfill operations and after closure. Leachate discharged from landfills is the main route for the release of the organic and inorganic contaminants commonly encountered in the refuse. Transport processes in landfills are associated with a high degree of uncertainty. While these processes are individually well understood and can be simulated reasonably well in a laboratory setting, their occurrence and interaction in landfills are still not fully comprehended (El-Fadel et al., 1997b[19]).

Substantial research and scientific evidence supports these mechanisms of pollution transfer and loss, but to ease the solution as a fast and simple scheme, several components require additional research and investigation. Therefore, the algorithms imbedded into the four essential components discussed above should be based on well-established and user-friendly models to estimate advection-diffusion-linear sorption with first order decay. A successful and practical pollution transfer and loss assessment tool should not demand that users fully understand the detailed theory behind the calculations, because, the real interactions between them are too complex. Although, the users should be trained enough to understand and assess the accuracy of the relative pollution transfer and loss estimates, and evaluate the benefit of adopting best management practices on underground water quality protection.

2. Transport Processes

2.1 Advection

- The process by which solutes are transported by the bulk of motion of the flowing ground water.
- Nonreactive solutes are carried at an average rate equal to the average linear velocity of the water.

2.2 Hydrodynamic Dispersion

- Tendency of the solute to spread out from the advective path

2.3 Diffusion of Contaminant

Ions (molecular constituents) in solution move under the influence of kinetic activity in direction of their concentration gradients.

- Occurs in the absence of any bulk hydraulic movement
- Diffusive flux is proportional to concentration gradient, in accordance to Fick’s First Law.
- Where \(D_m\) = diffusion coefficient (typically 1 x 10\(^{-5}\) to 2 x 10\(^{-5}\) cm\(^2\)/s for major ions in ground water)

\[
F = -D_m \frac{dc}{dx} \quad (1)
\]

- Fick’s Second Law - derived from Fick’s First Law and the Continuity Equation - called “Diffusion Equation”

\[
\frac{\partial C}{\partial t} = D_m \left( \frac{\partial^2 C}{\partial x^2} \right) \quad (2)
\]

2.4 Advection Dispersion Equation

Assumptions:
1) Porous medium is homogenous, 2) Porous medium is isotropic, 3) Porous medium is saturated, 4) Flow is steady-state and 5) Darcy’s Law applies

\[
F_x + \left( \frac{\partial y}{\partial x} \right) y = F + \left( \frac{\partial y}{\partial x} \right) y \quad (3)
\]

**Fig.1:** Mass balance element

2.5 Advection Dispersion Law

In the x-direction:

Transport by advection= \(\mathbf{v}_x n C dA\) units \(\frac{M}{T}\)

\[
(3)
\]
Transport by dispersion = \( nD_x \left( \frac{\partial C}{\partial x} \right) dx \) units \( \frac{M}{T} \) (4)

\( \bar{V} \) = average linear velocity, \( n \) = porosity (constant for unit of volume), \( C \) = concentration of solute and \( dA \) = elemental cross-sectional area of cubic element

\( D_x = \alpha_x \bar{V}_x + D_m \) (5)

Hydrodynamic Dispersion \( D_x \) caused by variations in the velocity field and heterogeneities.

\( \alpha_x = \) dispersivity \([L]\), \( D_m = \) Molecular diffusion.

\[ F_x = v_x nC - nD_x \left( \frac{\partial C}{\partial x} \right) \]  \( \tag{6} \)

- Flux = (mass/area/time)
- (-) sign before dispersion term indicates that the contaminant moves toward lower concentrations
- Difference in amount entering and leaving element = \( -\left( \frac{\partial F_x}{\partial x} \right) \)
- For nonreactive solute, difference between flux in and out = amount accumulated within element
- Rate of mass change in element = \( n \left( \frac{\partial C}{\partial x} \right) dx \) dy dz
- Equate two equations and divide by \( dV = dx \) dy dz:
- \[ -\left( \frac{\partial F_x}{\partial x} \right) + \left( \frac{\partial F_x}{\partial y} \right) + \left( \frac{\partial F_x}{\partial z} \right) = n \left( \frac{\partial C}{\partial x} \right) \]
- Substitute for fluxes and cancel \( n \):
- \[ -\left( \frac{\partial (F_x \bar{V}_x)}{\partial x} \right) + \left( \frac{\partial (F_x \bar{V}_y)}{\partial y} \right) + \left( \frac{\partial (F_x \bar{V}_z)}{\partial z} \right) + \left( \frac{\partial F_x}{\partial x} \right)(D_x \left( \frac{\partial C}{\partial x} \right)) + \left( \frac{\partial F_x}{\partial y} \right)(D_y \left( \frac{\partial C}{\partial y} \right)) + \left( \frac{\partial F_x}{\partial z} \right)(D_z \left( \frac{\partial C}{\partial z} \right)) = \frac{\partial C}{\partial x} \]  \( \tag{7} \)
- For a homogenous and isotropic medium, \( \bar{V} \) is steady and uniform. Therefore, \( D_x, D_y \) and \( D_z \) do not vary through space.

2.5.1 Advection-Dispersion Equation 3-D:

\[ \frac{\partial^2 C}{\partial t^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} \]

(8)

2-dimensional diffusion equation in transport equation is as follows:

\[ \frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} \]  \( \tag{12} \)

The finite difference which is chosen to solve the diffusion term is \( \beta \) formulation which is become the crank- Nicolson formulation with \( \beta = 0.5 \)
There are different ways of considering reaction terms and solving the ADRE. The solutions are presented in table 2.

![Table 1: Input parameter data to get 2D diffusion outputs](image)

### 3.2 A general form of finite volume algorithm for advection term

1-dimensional advection equation in transport equation is as follows. Where $C$ is Contaminant Concentration (mg/l), $U$, velocity (m/s), and $t$ indicates time (sec)

$$\frac{\partial C}{\partial t} = -\frac{\partial (Cu)}{\partial x}$$

(16)

Finite volume base formulation for all advection solution methods:

$$C_{j}^{n+1} = C_{j}^{n} \Delta x + C_{s_{j_{out}}}^{n-\omega t+1} - C_{s_{j_{out}}}^{n-\omega t+1}$$

(17)

$$C_{s_{j_{out}}}^{n} = C_{j}^{n} \Delta t$$

(18)

$$C_{s_{j_{out}}}^{n} = C_{j}^{n} \Delta t$$

(19)

![Fig. 4: Cell configuration in finite volume method (FVM)](image)

### 3.3. Finite Difference Algorithm for Decay (ADRE)

First order reaction term (Decay) in transport equation is as follows. $\lambda$ is First order reaction term coefficient, [T^{-1}], $C$ is dissolved concentration, [ML^{-3}] and $t$ is time, [T].

$$\frac{\partial C}{\partial t} = -\lambda C$$

(20)

Finite difference approximation of reaction term is:

$$\frac{C_{j}^{n+1} - C_{j}^{n}}{\Delta t} = -\lambda C_{j}^{n}$$

(21)

There are different ways of considering reaction terms and solving the ADRE. The solutions are presented in table 2.
4. Case Study Project

The landfill examined in this paper is located 16 km south of Beirut (Lebanon) and 4 km inland at an average altitude of 250 m above mean sea level. The landfill, once the site of an abandoned quarry, is planned for development over an area of 20–27 ha approximately, and receives 1700–2100 ton/day of waste generated from the Beirut area and its surroundings. The landfill will have an active life of 10 years and the final waste height may reach 100 m, making it one of the deepest in the world. Long term monthly meteorological data were taken from the Beirut International Airport (BIA) and the American University of Beirut (AUB) weather monitoring stations located within 15 and 20 km from the site, respectively. Total annual precipitation was 760 mm/year with average temperature, wind, and humidity of 21 °C, 4 m/s, and 63%, respectively (E. Bou-Zeid,[21], M. El-Fadel. [19]). The landfill which consists of three cells with different areas and capacities (Table 2).

5. Numerical Modeling Methodology

Leachate migration assessment typically involves two steps. First, leachate generation and infiltration through the landfill liner is quantified, then the migration of contaminants is modeled or measured in the porous subsurface until the point of compliance (the point where pollution level is to be assessed). The second step is presented in this paper. The theory and governing equations of flow and transport in porous media has been the subject of extensive work, particularly in the past two decades, in response to problems arising from subsurface contamination. All these models solve mass, momentum and heat transport equations; however, model capabilities and solution schemes may differ widely. In this study a numerical algorithm based on finite volume-finite difference methods was developed upon explicit - implicit solution has been employed using FORTRAN programming to reach an accurate and quick result.

6. Leachate Generation

In this paper, only the results that were used in subsurface transport simulations are presented. These results represent the baseline scenario likely to occur in view of the site characteristics. The landfill life was divided into three periods. The first period spans the first three years of the operational life of the site when cell number 1 is open; this cell has a different configuration than the rest of the landfill and is expected to produce more infiltration. The second period extends between years 3 and 10; cells 2 and 3 are operational during that period while cell 1 is closed and capped. Fig. 5-b is a cross sectional view of the landfill depicting the different layers in the three cells. The third period starts at year 10 when all cells are closed and the final cap of the landfill is installed. Figs. 6-a and b present the simulated leachate generation and infiltration into the subsurface from the landfill for the three periods, respectively.

<table>
<thead>
<tr>
<th>Table 2: Different solution of reaction term in ADRE</th>
</tr>
</thead>
</table>

1. Reaction term is solved separately as the same as advection and diffusion using simple FD method: $$C_{i+1}^{n} = (1 - \lambda \Delta t)^{\beta} C_{i}^{n}$$

2. Reaction term is solved separately as the same as advection and diffusion using \( \beta \) formulation of FD method:

$$\frac{C_{j}^{n+1} - C_{j}^{n}}{\Delta t} = -\lambda (1 - \beta) C_{j}^{n} - \lambda (\beta) C_{j}^{n+1} = (1 + \lambda (\beta) \Delta t)^{\beta} C_{j}^{n+1} = (1 - \lambda (1 - \beta) \Delta t)^{\beta} C_{j}^{n}$$

$$C_{j}^{n+1} = \left( \frac{(1 - \lambda (1 - \beta) \Delta t)}{(1 + \lambda (\beta) \Delta t)} \right)^{\beta} C_{j}^{n}$$

(22)

3. Reaction term is solved with diffusion term using simple FD method:

$$\left( \frac{-D(1 - \beta) \Delta x}{\Delta t} \right)^{\beta} C_{i+1}^{n+1} + \left( 1 + \frac{2D(1 - \beta) \Delta x}{\Delta t} \right)^{\beta} C_{i}^{n+1} + \left( \frac{-D(1 - \beta) \Delta x}{\Delta t} \right)^{\beta} C_{i-1}^{n+1} = \left( \frac{D(1 - \beta) \Delta x}{\Delta t} \right)^{\beta} C_{i+1}^{n} + \left( 1 + \frac{2D(1 - \beta) \Delta x}{\Delta t} \right)^{\beta} C_{i}^{n} + \left( \frac{D(1 - \beta) \Delta x}{\Delta t} \right)^{\beta} C_{i-1}^{n} + E(i)^{\beta}$$

(23)

4. Reaction term is solved with diffusion term using \( \beta \) formulation of FD method:

$$\left( \frac{-D(1 - \beta) \Delta x}{\Delta t} \right)^{\beta} C_{i+1}^{n+1} + \left( 1 + \frac{2D(1 - \beta) \Delta x}{\Delta t} + \beta \Delta t \right)^{\beta} C_{i}^{n+1} + \left( \frac{-D(1 - \beta) \Delta x}{\Delta t} \right)^{\beta} C_{i-1}^{n+1} = \left( \frac{D(1 - \beta) \Delta x}{\Delta t} \right)^{\beta} C_{i+1}^{n} + \left( 1 + \frac{2D(1 - \beta) \Delta x}{\Delta t} - (1 - \beta) \Delta t \right)^{\beta} C_{i}^{n} + \left( \frac{D(1 - \beta) \Delta x}{\Delta t} \right)^{\beta} C_{i-1}^{n} + E(i)^{\beta}$$

(24)
7. Subsurface Transport Simulation

7.1. Model Description

Programming is based on 2-dimensional numerical model for the analysis of dissolved material transport in subsurface transport modeling. The model simulates transport processes under steady state condition. It can simulate confined or unconfined, isotropic, homogeneous aquifers, fully or partially saturated media, single or multi phase systems.

7.2. Modeling Domain

The geologic formations at the site date back to the cretaceous age. They consist of weathered carbonaceous rocks including marls, marly limestones, dolomitic limestones, fossiliferous limestones and occasional sandstones. Perched groundwater was located beneath the site at depths as low as 15m below ground level; however, the main groundwater table lies at around 220 m below ground level, i.e., around 20–30 m above sea level. The general groundwater flow direction is westward towards the Mediterranean Sea with an approximate gradient of 0.05 (E. Bou-Zeid,[20], M. El-Fadel)[17]. This indicates that locations that might be adversely affected by the landfilling activity include water wells along the flow path from the landfill to the seashore. The nearest population center to the disposal site is located 2.5 km down gradient. Fig. 5-a,b presents a general schematic view of the simulated domain.

7.3. Modeling Process, Input Data, and Boundary Conditions

The selection of the contaminants to be modeled was based on the corresponding concentrations in site-specific leachate samples, susceptibility to natural attenuation, and drinking water standards (E. Bou-Zeid,[20], M. El-Fadel)[17]. An initial screening was conducted assuming no attenuation in the unsaturated zone. The screening revealed that Kjeldahl Nitrogen (K-N), Manganese (Mn), and Iron (Fe) would be the most critical indicators. Kjeldahl-N was retained as the main indicator since it is less affected by attenuation and retardation mechanisms than the other indicators and its concentration in the leachate remains relatively high (Kruempelbeck and Ehrig, 1999)[21]. Note that the Lebanese drinking water standards indicate a maximum allowable concentration of Kjeldahl-N of 1 mg/l (E. Bou-Zeid,[20], M. El-Fadel)[17]. The trends of the parametric sensitivity analysis for Kjeldahl-N should be valid for other pollutants.

7.3.1. The Unsaturated Zone

The flow and attenuation in the unsaturated zone are complex due to the heterogeneity of the topsoil and unsaturated rock zone beneath the landfill. To present a worst case scenario, chemical attenuation in the unsaturated zone was neglected. Therefore, all leachate and contaminants infiltrating to the subsurface are assumed to reach the groundwater table after the breakthrough time.

7.3.2. The Saturated Zone

The unconfined aquifer, which has an average thickness of 120 m approximately, is underlain by an aquiclude that forms a no-flow boundary condition for water and contaminants. The input parameters for the baseline scenario are summarized in Table 4.

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### Table 3: Areas and capacities of landfill cells

<table>
<thead>
<tr>
<th>Cell</th>
<th>Area (m²)</th>
<th>Expected waste capacities (ton)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>75,000-</td>
<td>1,362,167-</td>
</tr>
<tr>
<td></td>
<td>77,800</td>
<td>1,725,000-</td>
</tr>
<tr>
<td>2</td>
<td>52,609-</td>
<td>928,108-</td>
</tr>
<tr>
<td></td>
<td>138,000</td>
<td>5,580,000-</td>
</tr>
<tr>
<td>3</td>
<td>63,800-</td>
<td>1,009,725-</td>
</tr>
<tr>
<td></td>
<td>124,000</td>
<td>4,800,000-</td>
</tr>
<tr>
<td>Total</td>
<td>194,209-</td>
<td>3,300,000-</td>
</tr>
<tr>
<td></td>
<td>262,000</td>
<td>12,105,000-</td>
</tr>
</tbody>
</table>

---

**Fig. 5-a:** Cross sectional view of landfill operation
Leachate flow rate through the landfill base becomes subsurface infiltration. Subsurface infiltration decreases with capping of landfill cells (Fig. 4-b). An initial K-N concentration of 2500 mg/l in the subsurface infiltration is taken from (E. Bou-Zeid.[20], M. El-Fadel)[17]. Concentrations are assumed to decrease to reflect contaminant attenuation in the landfill (Table5). The X-axis is from the site towards the sea; the Y -axis is from the bottom to the top of the aquifer. Elements are geometrically uniform in the X and Y directions. The mesh size is $\Delta x = 10$ m, $\Delta y=2$ m and $\Delta t=0.2$ day. The bottom and vertical sides parallel to the stream wise velocity are set as no-flow boundaries. The top and upstream sides are inlet boundaries, while the downstream side is an outlet boundary.

8. Model Simulation Results

8.1. Base Line Modeling

Model simulations and a series of sensitivity analysis were conducted. Sensitivity analysis included variations in model parameters such as hydraulic gradient, aquifer hydraulic conductivity, source strength, diffusivity, longitudinal and transverse dispersivities. Fig 7-a),b),c),d) illustrates concentration distribution contours 5, 25, 50, and 75 years after the leachate reaches the ground water table. Note that the contour for the drinking water standard is far from the receptor location. This indicates that, for the base scenario, the potential contamination is confined within several hundred meters of landfill boundary.

Table.4: Input parameter to the simulating program

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Base value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thickness (m)</td>
<td>120</td>
</tr>
<tr>
<td>Saturated hydraulic conductivity(m/s)</td>
<td>$5 \times 10^{-4}$</td>
</tr>
<tr>
<td>Gradient (m/m)</td>
<td>30/6000</td>
</tr>
<tr>
<td>Total porosity (%)</td>
<td>15</td>
</tr>
<tr>
<td>Effective porosity (%)</td>
<td>12</td>
</tr>
<tr>
<td>Diffusivity in water (m²/year)</td>
<td>0.06</td>
</tr>
<tr>
<td>Longitudinal dispersivity (m²/year)</td>
<td>0.6</td>
</tr>
<tr>
<td>Transverse dispersivity (m²/year)</td>
<td>0.06</td>
</tr>
<tr>
<td>Background contaminant level (kg/m²)</td>
<td>0</td>
</tr>
</tbody>
</table>

Table.5: variation of leachate source strength versus time

<table>
<thead>
<tr>
<th>Time (yr)</th>
<th>Flow (m³/yr)</th>
<th>Kjeldahl-N concentration (mg/l)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0-3</td>
<td>0.022</td>
<td>2500</td>
</tr>
<tr>
<td>3-10</td>
<td>0.01</td>
<td>1500</td>
</tr>
<tr>
<td>$10^2$</td>
<td>0.005</td>
<td>1000</td>
</tr>
</tbody>
</table>

Fig.5-b: cross sectional of simulated domain

Fig.6: a) Leachate generation, b) Subsurface infiltration
8.2. Sensitivity Analysis

A sensitivity analysis was conducted to assess the effect of model parameters variation on contaminant transport simulation results. Dispersivities in the longitudinal and transverse direction were varied simultaneously. While higher groundwater velocities increase the speed of the plume spread, they increase dilution ratio and hence tend to decrease the concentration. The effect of increasing dispersivities (by a factor of 50) is to enhance transport in the transverse direction, this leads to a wide but short plume as depicted in Fig. 7-f. Increasing the hydraulic conductivity of the aquifer considerably reduces contaminant concentration due to increased dilution (Fig. 7-e). The temporal variation of the pollution levels is another aspect that is of significance when potential pollution from landfills is assessed. So the effect of varying model parameters on the history of concentrations was assessed. Fig. 8 shows a typical concentration history pattern. Dispersivity increments by a factor of 50 reduces concentrations. Doubling the source strength produces a predictable increase in concentrations. The increase in hydraulic gradient consistently reduces concentrations in
the vicinity of the site due to higher velocities and dilution ratios.

![Graph](image)

**Fig.8:** Sensitivity of simulated Kjeldahl-N concentration at the border of the landfill site to changes in input parameters.

9. Discussion and Conclusion

Accurate estimates of pollution loss require methods to quantify 1) pollution adsorbed to eroding sediments, 2) soluble pollution in runoff water, 3) soluble pollution in leaching water, and 4) pollution losses related to the specific pollution sources.

Although the accuracy of a pollution loss assessment is important, the relative ease of use by practitioners is essential. Thus, methods that estimate pollution loss related to the four mechanisms discussed should be based on established and user-friendly methods. The intended use of pollution loss assessment tools routinely interacting and control with land boundary conditions will minimize the contribution of pollution use on surface and groundwater quality.

The sensitivity of the model to variations in input parameters indicates that while higher groundwater velocities increase the speed of plume spread, they also decrease the dilution ratio and hence decrease the concentration. The most significant changes in pollution patterns were associated with changes in dispersivities, partition coefficient, source strength, and groundwater flow velocity. The unavailability of site-specific groundwater flow measurements to calibrate the model presents some limitations on the quality of the results.

References


