Boundary elements formulation of methane emission to the atmosphere from a landfill

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Abstract

The main objective of the present work is to develop a Boundary Element formulation for the problem of methane gas migration through a porous media, and its release into the atmosphere. This formulation is used as a basis for a numerical model of the physical process; in this study the methane at the porous media is a consequence of the degradation of waste material at a landfill.

1 Introduction

One of the most popular ways to dispose of domestic and industrial waste is to bury it under layers of soil, usually called landfill. A major concern derived from this disposing of waste is the generation of gases due to the degradation of waste materials in the repository. The primary source of gas production is the anaerobic microbial degradation of organic materials such as food waste, garden waste, paper, textiles, resins, bitumen, etc.

Of the various gas by-products, methane is the one of primary concern. Methane is produced by the action of micro-organisms on the degradable waste. The complex organic molecules in the above substances are broken down to smaller molecules. The process of forming methane is a two stage one. First the large organic molecules are broken down by hydrolysis to smaller, more soluble compounds. These include simple sugars, amino acids, fatty acids and alcohols. This stage is known as 'acidification'. The next stage involves further hydrolysis of the primary products to fatty acids. These are then metabolized by bacteria to produce methane.
Pressurization of the repository due to the internal gas production induces the emission of methane into the atmosphere. Methane is an important greenhouse gas since it is twenty times more reflective than carbon dioxide, and methane emissions have been increasing at a rate of about 1% per year.

Methane production and subsequent transport to the atmosphere and the soil surface is a complex process, in particular there is some uncertainty concerning the gas generation rate and its temporal variability. This initial modeling effort is based on a number of simplifying assumptions so that the most important mechanisms in the process are described adequately while maintaining relative simplicity in the model equations. The objective of this study is to examine some aspects of the methane migration problem using a 2-D vertical cross-sectional model. We focus on the gas flux within the repository and towards the atmosphere. We also investigate the sensitivity of the process to variations in material properties and model parameters.

2 Governing Equations

A mass balance leads to the following Diffusion-Convection equation

\[ D_x \frac{\partial^2 c}{\partial x^2} + D_y \frac{\partial^2 c}{\partial y^2} + \frac{\partial c u}{\partial x} - \frac{\partial c v}{\partial y} - k c + \phi - n \frac{\partial c}{\partial t} = 0 \]  

(1)

where the compressibility of the gas due to the confinement condition of the repository has been taken into account. Here, \( c \) in methane concentration, \( D_x \) and \( D_y \) are the diffusion coefficients of the gas through a porous media, \( u = (u, v) \) is the gas velocity vector through the porous media, \( k \) is the decay parameter, \( \phi \) is a source term and \( n \) is the material porosity.

The velocity of the gas is governed by the pressure gradient, the intrinsic permeability of the porous media and the viscosity of the fluid are expressed by Darcy’s Law, as

\[ u = -K \frac{\partial P}{\partial x} \quad \text{and} \quad v = -K \frac{\partial P}{\partial y} \]  

(2)

with \( K = k_r/\mu_{gas} \), \( k_r \) is the intrinsic permeability, \( P \) the gas pressure and \( \mu_{gas} \) the gas viscosity.

The gas pressure function is usually given by an empirical relation \( \text{(Narasimhan [1])} \), in terms of the methane concentration and two parameters \( a \) and \( d \)

\[ P = P_a + ac^d \]  

(3)

where \( P_a \) is the atmospheric pressure, generally taken to be zero. The exponent determines the curvature of the gas pressure function. For \( d = 1 \) the gas pressure reduces to the ideal gas equation with \( a = RT \), with \( R \) the gas constant and \( T \) the absolute temperature.
Substitution of equations (2) and (3) into equation (1) leads to the following non-linear governing partial differential equation for the gas concentration

\[ D_0 \frac{\partial^2 c}{\partial x^2} + D_0 \frac{\partial^2 c}{\partial y^2} - \left( K^* \frac{\partial c}{\partial x} \right) \frac{\partial c}{\partial x} - \left( K^* \frac{\partial c}{\partial y} \right) \frac{\partial c}{\partial y} - \left( K^* \left( \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} \right) + k \right) c + \phi - n \frac{\partial c}{\partial t} = 0 \] (4)

where, \( K^* = aK \), we have used the ideal gas model i.e., \( \gamma = 1 \), and assumed that the problem is isotropic \( D_x = D_y = D_0 \).

There are several empirical relations that relate the diffusion coefficient of one gas through another with the diffusion coefficient of a gas through a porous media, here we will use a relation given by Refsgaard et al. [2]

\[ \frac{D}{D_0} = 0.9n - 0.1 \] (5)

where \( D \) is the diffusion coefficient of one gas through another. For a porosity of \( n = 0.5 \), the ratio of the diffusion coefficient is 0.35.

The main objective of the present work is to develop an efficient and reliable numerical method to solve the problem of methane migration through porous media, and its release into the atmosphere.

### 3 Boundary Element Formulation

The Boundary Element Method (BEM) is a well established technique for the analysis of engineering problems, particularly those involving linear analysis. One of its main advantages is the considerable reduction in data preparation, in relation to domain methods, as only surface elements are necessary. The basis of the method is that a fundamental solution is used to take some or all of the terms in the governing equation to the boundary (see Brebbia et al. [3] and Brebbia and Dominguez [4]).

Further increase in the number of applications of BEM has been hampered by the need to operate with relatively complex fundamental solutions or the difficulties encountered when trying to extend the BEM to non-linear and time dependent problems, as is the case for the present problem. If those problems can be expressed in such a way that a simpler fundamental solution with a closed form, may be used and some terms expressed as domain integrals, considerable computational advantage may be obtained. In early boundary element analysis the evaluation of domain integrals was done using cell integration, a technique, which, whilst effective and general, made the method lose its boundary only nature introducing an additional internal discretization.

Several methods have been developed to take domain integrals to the boundary in order to eliminate the need for internal cells. One of the most effective to date
being the Dual Reciprocity Method (DRM). This method was introduced by Nardini and Brebbia [5], the method is general and straightforward to apply.

In order to apply the B.E.M. to find the solution of the non-linear partial differential equation for the gas concentration, we will re-write equation (4) in terms of the Laplacian linear operator, with the non-linear, the decay, the source and the non-permanent terms as nonhomogeneous terms of the Laplacian operator, i.e.

\[
\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} = \frac{1}{D_0} \left\{ \left( K^* \frac{\partial c}{\partial x} \right) \frac{\partial c}{\partial x} + \left( K^* \frac{\partial c}{\partial y} \right) \frac{\partial c}{\partial y} + \left( K^* \left( \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} \right) + k \right) c - \phi + n \frac{\partial c}{\partial t} \right\}. \tag{6}
\]

By applying the Green's representation formula for the Laplace equation and using the Dual Reciprocity method to take to the boundary the domain integral in the Green's formula, generated by the nonhomogeneous terms of equation (6), we found an integral equation formulation for the present problem with only boundary integrals (for more details on the DRM approach see Partridge et al [6]).

From the Green's representation formula, it is found that the methane concentration at a point "i", at the contour of the repository, is given by:

\[
\lambda_i c_i + \int_\Gamma q^* c d\Gamma - \int_\Gamma q c^* d\Gamma = \int_\Omega c^* b d\Omega \tag{7}
\]

where

\[
b = \frac{1}{D_0} \left\{ \left( K^* \frac{\partial c}{\partial x} \right) \frac{\partial c}{\partial x} + \left( K^* \frac{\partial c}{\partial y} \right) \frac{\partial c}{\partial y} + \left( K^* \left( \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} \right) + k \right) c - \phi + n \frac{\partial c}{\partial t} \right\},
\]

here \(c^*\) is the fundamental solution of the 2-D Laplace equation

\[
c^* = \frac{1}{2\pi} \log \frac{1}{r}
\]

and \(q^* = \partial c^*/\partial n\). Notice that in equation (7) all the integrals are over the boundary with the exception of the one corresponding to the term \(b\). The constants \(\lambda\) have values between 1 and 0, being equal to 1/2 for smooth boundaries. It is also important to point out that the above equation holds for points inside the repository, in this case \(\lambda_i = 1\).

In order to express the domain integral in equation (7) in terms of equivalent boundary integrals, a DRM approximation is introduced. The basic idea is to expand the "b" term in the form,

\[
b_i = \sum_{j=1}^{N+L} \alpha_j f_{ij}. \tag{8}
\]
where \( b_i \) is the value of the function \( b \) at node \( i \). The \( f_{ij} \) are approximating functions and the \( \alpha_j \) unknown coefficients. The approximation is done at \((N + L)\) nodes, \( N \) boundary nodes and \( L \) internal nodes. Previous work on dual reciprocity has shown (see Partridge et al. [6]), that although a variety of functions can in principle be used as a basic approximation function, best results are normally obtained with simple expansions, the most popular of which is \( f = 1 + R \), where \( R \) is the distance between pre-specified fixed collocation points, \( y^m \), and a field point \( x \) where the function is approximated, i.e. \( R = |x - y^m| \).

With this approximation for the nonhomogeneous term, "\( b \)" , the domain integral in equation (7) becomes

\[
\int \mathbf{c}^*b d\Omega = \sum_{j=1}^{N+L} \alpha_j \int c^*f_{ij} d\Omega
\]  

(9)

To reduce the last domain integral in the above equation to equivalent boundary integrals, let us define a new auxiliary nonhomogeneous Laplacian field, \( \tilde{\mathbf{c}}_j \), for each collocation point "\( j \)”, in the following way:

\[
\nabla^2 \tilde{\mathbf{c}} = f, 
\]

(10)

which particular solution for \( f = 1 + R \) is given by:

\[
\tilde{\mathbf{c}} = \frac{R^2}{4} + \frac{R^3}{9}
\]

Applying the Green’s formula to the non-homogeneous Laplacian field \( \tilde{\mathbf{c}} \), at a point "\( i \)”, we obtain:

\[
\int \int c^*f_{ij} d\Omega = \lambda_i \tilde{c}_i + \int \int q^*\tilde{c} d\Gamma - \int \tilde{q} c^* d\Gamma
\]

(11)

Substituting the last equation into equation (9), the domain integral can be recast in the form

\[
\int \mathbf{c}^*b d\Omega = \sum_{j=1}^{N+L} \left\{ \alpha_j \left( \int \tilde{c}_j q^* d\Gamma - \int \tilde{q}_j c^* d\Gamma + \lambda_i \tilde{c}_i \right) \right\}
\]  

(12)

and using the resulting expression in equation (7), one finally arrives at a boundary only integral representation formula for the methane concentration

\[
\lambda_i c_i - \int q_i^* \left( \frac{\partial c}{\partial n} \right) d\Gamma + \int q_i^* c d\Gamma =
\sum_{j=1}^{N+L} \left\{ \alpha_j \left( \int \tilde{c}_j q_i^* d\Gamma - \int \tilde{q}_j c_i^* d\Gamma + \lambda_i \tilde{c}_i \right) \right\}
\]  

(13)

The coefficients \( \alpha_j \) in the above equation can be calculated evaluating equation (8) at all \((N + L)\) nodes, i.e.

\[
\mathbf{b} = \mathbf{F} \mathbf{\alpha}
\]

\[
\mathbf{\alpha} = \mathbf{F}^{-1} \mathbf{b}
\]  

(14)

and therefore, its evaluation depends on the DRM approximation of each of the terms defining the nonhomogeneous term "\( b \)".
4 Dual Reciprocity Approximation of the Nonhomogeneous Term

1) The gradient of the concentration:

At this point it should be remembered that the basic approximation of the DRM technique is

\[ b = F\alpha \]  

(15)

A similar equation may be written for \( c \)

\[ c = F\beta \]  

(16)

where \( \beta \neq \alpha \). Differentiating equation (16) produces

\[ \frac{\partial c}{\partial x} = \frac{\partial F}{\partial x}\beta \]  

(17)

Rewriting equation (16) as

\[ \beta = F^{-1}c, \]  

(18)

and substituting it into equation (17), we obtain:

\[ \frac{\partial c}{\partial x} = \frac{\partial F}{\partial x}F^{-1}c \]  

(19)

A similar expression can be written for the derivative in the \( y \) direction.

\[ \frac{\partial c}{\partial y} = \frac{\partial F}{\partial y}F^{-1}c \]  

(20)

2) The Laplacian of the concentration:

Differentiating equation (17) one obtains

\[ \frac{\partial^2 c}{\partial x^2} = \frac{\partial^2 F}{\partial x^2}\beta \]  

(21)

Substituting equation (18) into the above equation, we obtain

\[ \frac{\partial^2 c}{\partial x^2} = \frac{\partial^2 F}{\partial x^2}F^{-1}c \]  

(22)

Similarly

\[ \frac{\partial^2 c}{\partial y^2} = \frac{\partial^2 F}{\partial y^2}F^{-1}c \]  

(23)

It should however be noted that in the case of expressions (22) and (23) the approximation function, \( f = 1 + R \), cannot be used, as its second derivative is singular. For this reason, the function \( 1 + R^3 \) is used in the approximation of the Laplacian, instead of the \( 1 + R \) used for the other terms (for more detail on the DRM approximation for higher differential operators see Partridge et al [6]).

3) Time derivative:
Using a simple finite-difference representation for the time derivative one obtains

\[
\frac{\partial c}{\partial t} = \frac{1}{\Delta t}(c(t) - c_0)
\]

(24)

where \(c(t)\) are the nodal values of \(c\) at time \(t\) and \(c_0\) are the values at time \(t - \Delta t\).

For the first time step \(c_0 = c(t = 0)\).

5 The Treatment of non-linear terms

In order to deal with the non-linear terms appearing in equation (6), a standard linear approximation will be used, where the approximated gradient and Laplacian of the concentration will be written as the diagonal matrices \((V_x, V_y)\) and \(K_0\), containing the values of the differential operators \((K^*\partial c/\partial x), (K^*\partial c/\partial y),\) and \(K^*(\partial^2 c/\partial x^2 + \partial^2 c/\partial y^2)\) for a priori estimation of the concentration, \(\tilde{c}_j\), at the interpolation nodal points, at each time step, thus

\[
\begin{align*}
\left( K^* \frac{\partial c}{\partial x} \right) \frac{\partial c}{\partial x} &= V_x \frac{\partial F}{\partial x} F^{-1} \tilde{c}, \\
\left( K^* \frac{\partial c}{\partial y} \right) \frac{\partial c}{\partial y} &= V_y \frac{\partial F}{\partial y} F^{-1} \tilde{c},
\end{align*}
\]

(25)

(26)

and

\[
K^* \left( \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} \right) c = K_0 c
\]

(27)

where

\[
V_x = \frac{\partial F}{\partial x} F^{-1} \tilde{c},
\]

(28)

\[
V_y = \frac{\partial F}{\partial y} F^{-1} \tilde{c},
\]

(29)

and

\[
K_0 = \left( \frac{\partial^2 \tilde{F}}{\partial x^2} + \frac{\partial^2 \tilde{F}}{\partial y^2} \right) \tilde{F}^{-1} \tilde{c}
\]

(30)

where \(\tilde{F}\) is the matrix representation of the interpolation function \(1 + R^3\).

The above expression for the non-linear terms makes the procedure iterative, since it is necessary to assume a priori estimation of the concentration at each time step, \(\tilde{c}\), at the interpolation nodal points, in order to evaluate the concentration \(c(t)\), using the corresponding boundary only integral equation discussed before. Letting the evaluated \(c(t)\), for a given time, becomes \(\tilde{c}\) for a new iteration the process is continued until convergence is obtained at each time step. In our numerical examples we have done around 10 to 15 iterations at each of the initial time steps, after that only few iterations, between 3 to 5, where needed to satisfy the convergence requirement of 1% local error.
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With this approximation for the non-linear terms, the terms given by equations (25) and (26), at each iteration for a given time step, are treated as the usual convective terms in the Diffusion-Convection equation for an incompressible fluid, and the term given by equation (27) as an apparent decay term, with a variable velocity field \((V_x, V_y)\) given by equation (28) and (29) and a variable decay coefficient given by equation (30), respectively.

In this way at each iteration for a given time step, the function "b" will be approximated by the following expression:

\[
b = \frac{1}{D_0} \left\{ V_x \frac{\partial F}{\partial x} F^{-1} + V_y \frac{\partial F}{\partial y} F^{-1} + (K + K_0) + \frac{n}{\Delta t} \right\} c(t) \]

\[- \frac{1}{D_0} \left( \frac{n}{\Delta t} c_0 + \phi \right) \quad (31)\]

Substitution of the above expression for "b" into equation (14) leads to the final expression for the coefficient \(a_j\) in equation (13).

6 Numerical Examples

To test the numerical model developed in this work, we analyzed a hypothetical square repository with an initial methane concentration of 0.30, with zero flux boundary condition at the bottom and at the two sides of the repository and atmospheric pressure, \(P = P_a = 0\), at the land surface. The parameters of the model was taken from the works of Hughes and Spink [7], Peyton and Schroeder [8] and Mishra et al. [9], and they are \(D_0 = 0.154 \text{ m}^2/\text{d}, k = 10^{-12}\text{m}^2, K = k_r/\mu_{\text{gas}} = 0.23210^{-2}\text{m}/\text{d}, K^* = 0.5\text{m}^2/\text{d}\) and \(n = 0.5\). In figure 1, we present how the concentration profile change with time, for \(t = 1, 2, 3, 4\) and \(5\) days, when the decay and source terms are taken to be zero. In figure 2, we compare the concentration profile, at day five, for the previous case and the case when the middle of the land surface is considered to be closed, with dimensionless closed length of \(d/L = 3/9\), with \(L\) as the total length of the land surface. Figure 3 give how the flow discharge, of gas methane, through the atmosphere change with time, for the two previous cases, and in figure 4 we show how the concentration profile depends on the source term. For the last case considered, with a source coefficient of \(\phi = 0.005\), a flow discharge of \(q = 1.638\) at day five was obtained. From comparison of these results, it can be concluded that the main effect of the variation of the parameters considered, upon the discharge to the atmosphere, is predominantly during the initiation of the process, after some time its effects are not significant. The above statement makes critical the effectiveness of any gas emission control method.

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References


Figure 1: Concentration profile at different times for the case of total open land surface, with zero decay and source terms.
Figure 2: Comparison of the concentration profile between the cases of total open land surface and partially closed land surface (with zero decay and source terms), at day five.
Figure 3: Comparison of the flow discharge through the atmosphere between the cases of total open land surface and partially closed land surface (with zero decay and source terms), at day five.
Figure 4: Comparison of the concentration profile between the case of zero source term and the case of source coefficient $\phi = 0.005$, at day five.