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Numerical model of compressible gas flow in soil pollution control

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Abstract: Based on the theory of fluid dynamics in porous media, a numerical model of gas flow in unsaturated zone is developed with the consideration of gas density change due to variation of air pressure. This model is characterized of its wider range of availability. The accuracy of this numerical model is analyzed through comparison with modeling results by previous model with presumption of little pressure variation and the validity of this numerical model is shown. Thus it provides basis for the designing and management of landfill gas control system or soil vapor extraction system in soil pollution control.

Keywords: numerical model; compressible gas; landfill gas; migration; soil vapor extraction; pollution control

Introduction

Landfill gas will be generated after one year of landfilling of municipal solid waste. The components of landfill gas are mainly CH_4, CO_2, with additional some trace constitutes such as N_2, H_2, H_2S, and volatile organic compound and so on. Landfill gas will be accumulated in the landfill and be released. Thus it will result in serious safety and health hazards (Department of Environment, 1997; Theison, 1993). Moreover in soil pollution remediation, technique of soil vapor extraction is often adopted, in which extraction wells and injection wells (or air vents) are used to control gas migration and to collect gases for treatment (Pedersen, 1991).

The emission of noxious gas and solute from sanitary landfills and other waste disposal areas can present a significant hazard to the environment if not properly controlled. Transport of harmful vapors from hazardous waste spills or disposal sites through soil into areas has also been recognized as serious environmental health hazard. Implementing such measures is expensive, and with limited resources it is important to know quantitatively the underlying mechanisms involved and the effect of various strategies on them. In order to get the harmful gas controlled and mitigate the environmental pollution, measures must be taken and it is often important to know the extent to which the gas will be transported through soil at some time in the future. However it is practical or even feasible to make these judgements. Thus mathematical models can be used to predict gas migration. This will provide the theoretical basis for designing gas controlling system for landfill or venting system for soil pollution remediation.

Topic of modeling of gas migration in soil from landfills or from soil vapor extraction system is discussed by Metcalfe *et al*. (Metcalfe, 1987), Massmann *et al*. (Massmann, 1989; 1994), Young (Young, 1989), Johnson *et al*. (Johnson, 1990) and a variety of mathematical models with varying levels of complexity have been used to describe gas migration from landfills or in soil vapor extraction process. All of their work is based on fluid dynamics in porous media. Massmann *et al*. (Massmann, 1989) and Johnson *et al*. (Johnson, 1990) applied groundwater model in vapor extraction system design, in which transient analytical model were developed and Johnson *et al*. developed a model just based on the Theison solution developed for groundwater flow in confined aquifer, assuming one-dimensional, radial flow in a homogeneous and isotropic field. Young (Young, 1989) also derived semi-analytical model for landfill gas extraction. In the work of Metcalfe *et al*. (Metcalfe, 1987) and Massmann *et al*. (Massmann, 1994), mathematical model for gas transport were also developed. The work of Massmann *et al*., Johnson *et al*.

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and Young were done all under assumption of small variation of gas pressure, which results in linearization of the differential equation. In our study, numerical model for gas migration from landfill or from soil vapor extraction system is developed in consideration of gas compressibility comprehensively. Solutions of this model are compared to those of previous model with assumption of small variation of gas pressure. The extent of validity and availability of the previous model are analyzed through comparison in cases of different gas pressure variation. And the validity and availability of this numerical model are shown.

1 Mathematical model for compressible gas migration

1.1 Governing equation of gas migration in porous media

Under assumption of negligible distortion of media and steady water movement, there is following governing equation for gas migration based on fluid dynamics(Bear, 1972):

$$S_G n_e \frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \vec{V}) + \rho q, \tag{1}$$

where S_G is the ratio of gas to porosity; n_e is the effective porosity; ρ is the gas density(kg/m^3); t is the time(d); $\vec{V}$ is Darcy velocity(m/d); q is the source, i.e. gas generation rate(1/d); ∇ is Hamiltonian operator.

If ideal gas is assumed, then

$$\rho = \frac{W_m p}{RT}, \tag{2}$$

where W_m is the molecular weight(kg/mole); p is the gas pressure(Pa); R is the ideal gas constant(m^3·Pa/(mol·K)); T is the temperature(K).

Based on fluid dynamics, Darcy velocity can be written as:

$$\vec{V} = -\frac{\bar{k}}{\mu}(\nabla p + \rho g \nabla z), \tag{3}$$

where $\bar{k}$ is the permeability tensor(m^2); g is the acceleration of gravity(m/s^2); μ is the viscosity of gas (Pa·s); z is the location in vertical direction(m).

Substitute Eq.(2) and Eq.(3) into Eq.(1), then

$$S_s \frac{\partial p}{\partial t} = \nabla \cdot \left(\rho \frac{\bar{k}}{\mu}(\nabla p + \rho g \nabla z)\right) + \rho q, \tag{4}$$

where $S_s = \dfrac{S_G n_e W_m}{RT}$.

Eq.(4) is governing equation for compressible gas migration and it is a nonlinear partial differential equation since gas density ρ in the right side of Eq.(4) is the function of gas pressure p. To completely define the problem, Eq.(4) must be constrained by initial and boundary conditions and they make up mathematical model for compressible gas migration.

The difference between this model and previous model(Metcalfe, 1987; Massmann, 1989; Young, 1989) lies in assumption of gas density. In previous model, average gas density is assumed in right side of Eq.(4) in order to linearize the differential equation though ideal gas Eq.(2) is coupled in the left side and thus there must be innegligibe error in case of significant variation of gas pressure. In our study, the nonlinear partial differential Eq.(4) is solved by numerical techniques through iteration by applying Eq.(2).

1.2 Initial and boundary conditions

In order to establish mathematical model for compressible gas migration, initial and boundary conditions are needed to be coupled in. The initial and boundary conditions are

(1) Initial condition

$$p\big|_{t=0} = p_0, \tag{5}$$

where p_0 is the prescribed initial condition of pressure.

(2) Boundary conditions

$$p|_{\Gamma_1} = p_1, \tag{6}$$

$$-\vec{n}\cdot\left(\frac{k}{\mu}(\nabla p + \rho g \nabla z)\right)\Big|_{\Gamma_2} = q_2, \tag{7}$$

where Γ_1 is Dirichlet boundary; Γ_2 is Cauchy boundary; p_1 is the prescribed Dirichlet function value of pressure; q_2 is the prescribed Cauchy flux; $\vec{n}$ is the outward unit vector normal to the boundary.

The governing Eq.(4), and initial and boundary conditions, i.e., Eq.(5) – (7) make up mathematical model for compressible gas migration.

2 Numerical model for compressible gas migration

The governing Eq.(4) is a nonlinear partial differential equation. In order to get solution, numerical method is adopted. Usually the real problem can be generalized into two dimensional issues and thus in the following sectional two dimensional problem is assumed.

Discretize the domain of interest Ω, an element can be either quadruple or triangle. It is assumed that m element and n nodes are formed after discretization. Substitute p by its approximation, i.e.,

$$p \cong \hat{p} = \sum_{i=1}^{n} p_j(t) N_j(x,z), \tag{8}$$

where N_j is the basis function of node j; p_j is the pressure at node j.

Based on variational principle and Galerkin finite element method, variational equation corresponding to Eq.(4) – (7) can be derived first, substitute pressure approximation(Eq.(8)) into variational equation and thus finite element equations can be derived

$$[M]\left\{\frac{\mathrm{d}p}{\mathrm{d}t}\right\} + [S]\{p\} = \{G\} + \{Q\} + \{B\}, \tag{9}$$

where $\{\mathrm{d}p/\mathrm{d}t\}$ and $\{p\}$ are the column vectors containing the values of $\mathrm{d}p/\mathrm{d}t$ and p respectively at each node, $[M]$ is the mass matrix resulting from storage term; $[S]$ is the stiff matrix resulting from the action of conductivity. $\{G\}$, $\{Q\}$ and $\{B\}$ are the load vectors from the gravity force, internal source/sink and boundary conditions respectively. They are expressed as follows:

$$\begin{cases} M_{ij} = \sum\limits_{e\in M_e} \int\limits_{\Omega_e} N_\alpha^e S_s N_\beta^e \mathrm{d}\Omega; \\ S_{ij} = \sum\limits_{e\in M_e} \int\limits_{\Omega_e} (\nabla N_\alpha^e)\cdot \rho \frac{k}{\mu}(\nabla N_\beta^e)\mathrm{d}\Omega; \\ G_i = -\sum\limits_{e\in M_e} \int\limits_{\Omega_e} (\nabla N_\alpha^e)\cdot \rho^2 \frac{\bar{k}}{\mu} g \nabla z \mathrm{d}\Omega; \\ Q_i = \sum\limits_{e\in M_e} \int\limits_{\Omega_e} (\nabla N_\alpha^e)\cdot \rho q \mathrm{d}\Omega; \\ B_i = -\sum\limits_{e\in N_{se}} \int\limits_{B_e} N_\alpha^e \vec{n}\cdot \rho\left(-\frac{k}{\mu}(\nabla p + \rho g \nabla z)\right)\mathrm{d}B, \end{cases} \tag{10}$$

where Ω_e is the domain of element e; M_e is the set of elements that have a local side α-β coinciding with the global side i-j; N_α^e is α-th local basis function of element e(corresponding to global node i); B_e is the length of boundary segment e, N_{se} is the set of boundary segments that have a local node coinciding with the global node i.

There is pressure derivative to time i.e., $\mathrm{d}p/\mathrm{d}t$, in Eq.(9). Thus, finite difference method are typically used in the approximation of the time derivative. Substitute time difference into time derivative, then Eq.(9) can be written as following algebra equations

$$[T]\{p\} = \{Y\}, \tag{11}$$

where $[T]$ is the matrix, $\{p\}$ is the unknown vector and represents the values of discretized pressure field at current time, and $[Y]$ is the load vector. Take for example, when back difference formulation is adopted in Eq.(11), $[T]$ and $[Y]$ represent the following

$$\begin{cases} [T] = [M]/\Delta t + [S] \\ \{Y\} = [M]\{p\}_t/\Delta t + \{G\} + \{Q\} + \{B\}. \\ \{p\} = \{p\}_{t+\Delta t} \end{cases} \tag{12}$$

Eq.(11) is finite element equations of mathematical model for compressible gas migration in soil, i.e., Eq.(4) and Eq.(7). Numerical solution can be obtained by solving Eq.(11).

This numerical model is not only applicable to sectional view two dimensional issues but also to plan view two dimensional issues. Just set the item of $\{G\}$ in Eq.(9) to be zero(neglecting gravity item) when it is used for plan view two dimensional issue. Based on the finite element Eqs.(11) – (12) and Eqs.(9) – (10), computer source code FEMGS2 (finite element method for compressible gas migration in 2 dimension) is compiled and it serves as tools for the following analysis.

3 Comparison analysis of numerical models

In comparison analysis of numerical models, this numerical solution serves as accurate solution for the mechanism of gas compressibility is taken into account comprehensively. Previous model solution is compared with this numerical solution. In case study, geological property parameters and gas monitoring data of Ottawa Street Landfill is adapted(Metacafe, 1987). Comparisons between this numerical solution and previous model solution are made under different pressure variations resulting from venting, such as venting as active landfill gas control system, pumping as barrier preventing landfill gas from entering adjacent area, and as venting for soil pollution remediation by oil.

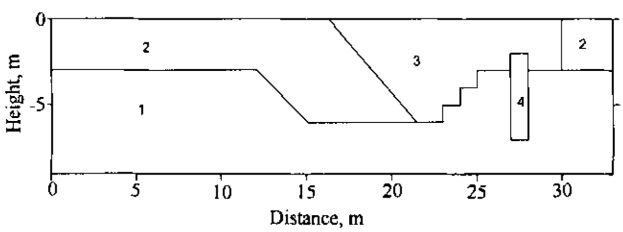

Fig.1 Geological structure around Ottawa Street Landfill in Canada
1.sand; 2.sand loam; 3.loam; 4.vent

The soils around Ottawa Street Landfill site are sand, sand loam and loam. The geological structure and soil parameters are presented in Fig. 1 and Table 1. Fig. 1 is soil profile around Ottawa Street Landfill, the top and bottom coincide with ground surface and the water table, respectively; landfill is at the left side stretching approximately 12*m* from the left and a gas interceptor vent is positioned 27m to the left boundary aiming at being a barrier preventing landfill gas from migrating forward; the right boundary is chosen 5m beyond the gas interceptor vent. The length of modeled profile is 33m and the depth is 9m. Quadrilateral elements and triangular elements are discretized, generating 340 nodes and 306 elements. The parameters used in modeling are as follows:

$W_m = 28.6165 \times 10^{-3}$ kg/mol; $R = 8.3134$ $(m^3 \cdot Pa)/(mol \cdot K)$; $T = 293.15$ K; $\rho = 1.13216$ kg/m^3; $\mu = 1.8 \times 10^{-5}$ Pa · s.

Table 1 Soil parameters around Ottawa Street Landfill

Soil type	Permeability, m^2	Porosity	Water content
Sand	5×10^{-12}	0.35	0.05
Sand loam	1×10^{-13}	0.40	0.10
Loam	1×10^{-14}	0.45	0.25

Results of comparison between this numerical model solution and previous model solution are shown in Fig.2, 3 and Table 2. Fig.2 and 3 show comparison between two model solutions under relatively big pressure variation and small pressure variation. When pressure variation in the modeled gas flow system is 51477 Pa, i.e., about half an atmosphere pressure, the error resulting from previous model is quite large, 9447 Pa, 18.35% of gas pressure variation in the modeled system; when pressure variation is 11637 Pa, approximately 0.1 of atmosphere pressure, the error from previous model is relatively large, 360 Pa, 3.09% of pressure variation; when pressure variation is 1528 Pa, about 0.015 of atmosphere pressure, the error from previous model is relatively small, 13 Pa, 0.85% of pressure variation. Thus if landfill gas control system is the system of gas collection inside the landfill by pumping, pressure variation in the system is small, usually less than 4000 Pa, the error of previous model is relatively small and can be neglected. And if venting is used for soil pollution remediation in soil vapor extraction or pumping is positioned beyond landfill as barrier, gas pressure variation is relatively large, the error of previous model can not be neglected for pressure variation can be 0.1 atm or even bigger according to Anderson(Anderson, 1994) and Hinchee (Hinchee, 1997) and 12552 Pa vacuum pressure can be produced by blower according to Pedersen (Pedersen, 1991).

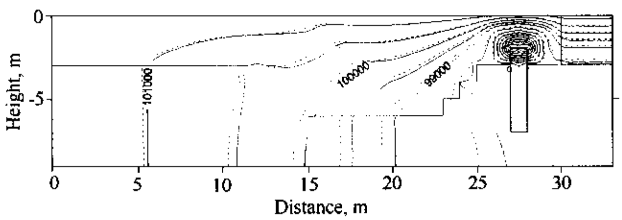

Fig.2 Gas pressure distribution in case of relative big pressure variation (pressure variation of 11637 Pa)

Table2 Comparison of numerical modeling results

Pressure variation, Pa	Max error, Pa	Average error, Pa
51477	9447	1409.5
11637	360	83.0
5172	76	23.3
1528	13	4.0
289	10	0.8

4 Conclusion

A numerical model for compressible gas migration in porous media is developed for soil pollution control taking into account of gas compressibility comprehensively based on fluid dynamics in porous media and it is more comprehensive and of wide application. Comparison between this numerical model solution and previous model solution are made and analyzed. Results show that in case of landfill gas collection, pressure variation is relatively small, usually less than 4000 Pa, the error from previous model can be neglected, while in case of venting in soil vapor extraction as for soil pollution remediation or as barrier beyond landfill, pressure variation can be 0.1 of atmosphere pressure or even larger, the error from previous model is relatively big and can not be neglected. Thus this numerical model of compressible gas migration must be used. It can provide more reasonable basis for environmental impact assessment of landfill gas migration, soil pollution remediation and for designing or management of pollution control system.

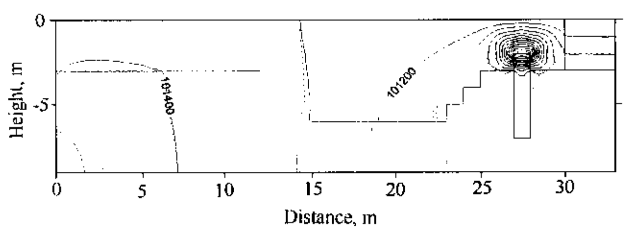

Fig.3 Gas pressure distribution in case of relative small pressure variation (pressure variation of 1528 Pa)

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