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New development in the modelling of the coupling processes in landfills involving discontinuous flow and carbon-nitrogen flow

Shi-Jin Feng[a,b*], Xiao-Wei Zhang[a], Qi-Teng Zheng[a], Shao-Jie Wu[a], Yong Zhao[a]

[a] *Department of Geotechnical Engineering, Tongji University, 200092 Shanghai, China*

[b] *Key Laboratory of Geotechnical and Underground Engineering of the Ministry of Education, Tongji University, Shanghai 200092, China*

* *Corresponding Author, Email: 08qitengzheng@tongji.edu.cn*

ABSTRACT

The coupling processes in unsaturated regions of anaerobic and aerobic landfills have been widely studied and modelled. However, the previous studies cannot address two new problems in practice: a large quantity of landfill gas (LFG) generated and accumulated below leachate level, and the quantitative prediction of the stabilization of three-phase waste under aeration, especially leachate. Thus, this paper introduce the new development in the modelling of the coupling processes in landfills. Firstly, a liquid-gas discontinuous migration model considering bubble formation in the highly saturated area is developed, including LFG bubble formation and two-fluid flow. This model can be used to reveal the mechanism of LFG accumulation, leachate uplift and leachate-gas discontinuous flow. Secondly, new sub-models of methane oxidation, nitrification and denitrification, transports of new solutes and non-equilibrium solid-liquid heat transfer, and nonuniform deformation caused by creep and biodegradation are added to the aerobic landfill multi-field coupled models. This model can be used to study the accelerated stabilization of landfilled waste from solid, gas and liquid phases, and the flows of carbon and nitrogen elements among different phases and components under aeration.

Keywords: Landfill; Leachate-gas discontinuous flow; Stabilization; Carbon-nitrogen flow.

1 INTRODUCTION

In the past few decades, the organic content and water content of municipal solid waste in developing countries such as China are higher than those in other developed countries, leading to higher pore pressure and leachate level during the degradation process of waste, which seriously threatens the stability of landfills. In order to accelerate the degradation of waste and promote the stabilization of landfills, the concept of aerobic landfills was put forward and has been successfully applied (Hrad and Huber-Humer, 2017). Predicting the stabilization process of aerobic landfills is of great significance for the design and operation of landfills.

Waste biodegradation is a complex process, which is affected by many environmental factors such as oxygen concentration and temperature. In the process of biodegradation, landfill gas, leachate and heat will be generated during the biodegradation process, which will have an important impact on the liquid-gas migration, heat transfer and settlement deformation inside the waste. There are also complex coupling influence mechanisms among various physical fields. In order to reveal the coupling mechanism of landfilled waste, some coupling models of anaerobic landfills and aerobic landfills have been proposed. For example, Ishimori et al. (2011) proposed a bio-water-thermal coupling model to simulate the stabilization of waste in semi-aerobic landfills, which considered both aerobic and anaerobic biodegradation but ignored the flow of leachate. Fytanidis and Voudrias (2014) proposed a liquid-air migration model for unsaturated waste to simulate the degradation process of organic matter and temperature changes, but did not consider liquid-gas migration in saturated areas. In fact, in saturated areas below the leachate level, the biodegradation of waste is still continuing. Landfill gas (LFG) generated by degradation will accumulate and flow in the form of bubbles, inducing high gas pressure below the leachate level. The distributions of leachate and LFG in both unsaturated and highly saturated regions of landfills will then be significantly affected, together with the stability of landfill slopes. Thus, the first part of this paper is to establish the liquid-gas migration model considering bubble generation in the highly saturated area of the landfill, including LFG bubble formation model and two-fluid model to reveal the accumulation of LFG bubble and the mechanism of leachate-gas discontinuous flow.

At present, most aerobic landfill models mainly consider anaerobic-aerobic biodegradation, leachate-gas flow, gas component transport and heat transfer, but ignore landfill deformation and solute transport. In the second part of this paper, further work has been carried out on the basis of the multi-field coupled model framework of aerobic landfill proposed by Zheng et al. (2022). New sub-models of methane oxidation, nitrification and denitrification, transports of generated solutes, non-equilibrium solid-liquid heat transfer, and creep-biodegradation deformation are added to allow the prediction of the stabilization process of aerobic landfills.

2 LIQUID-GAS DISCONTINUOUS MIGRATION MODEL BELOW LEACHATE LEVEL

Below the leachate level, waste biodegradation and LFG generation continue, forming a large quantity of LFG bubbles. Most previous studies focused on the migration of liquid and gas above the leachate level (i.e., unsaturated areas), without considering the underwater part. They cannot accurately describe the high gas pressure as observed at the deep-buried waste in practice, and hence significantly over- or under-estimate the stability of landfills. Thus, a liquid-gas migration model considering bubble formation and accumulation in highly saturated area was established, including bubble generation model and two-fluid model.

2.1 Bubble generation model in highly saturated area

The bubble generation model in highly saturated area includes liquid continuity equation, porous medium bubble generation model and bubble force equilibrium model.

2.1.1 Liquid continuity equation

In the stage of bubble development, the liquid phase was regarded as a continuous fluid, and the generation of LFG bubbles will change the pressure distribution of leachate. In order to describe the pressure distribution of liquid phase caused by bubble generation, the liquid phase continuity equation is introduced. In the unit volume of landfill, the volume of liquid outflow is equal to the sum of the volume of liquid inflow and the volume of bubbles generated. The formula is as follows:

$$(u_1+\frac{\partial u_1}{\partial z}\mathrm{d}z)\mathrm{d}x\mathrm{d}y\mathrm{d}t=u_1\mathrm{d}x\mathrm{d}y\mathrm{d}t+\frac{\partial \theta_\mathrm{g}}{\partial t}\mathrm{d}x\mathrm{d}y\mathrm{d}z\mathrm{d}t \tag{1}$$

$$\frac{\mathrm{d}\theta_\mathrm{g}}{\mathrm{d}t}=-k_\mathrm{w}\frac{\partial^2 h_1(z,t)}{\partial z^2} \tag{2}$$

where u_1 is the one-dimensional (z direction) flow velocity of the liquid phase ; θ_g is the volume fraction of the generated gas ; k_w is the liquid permeability coefficient ; h_1.is the liquid head pressure.

2.1.2 Bubble generation model in highly saturated porous media

To describe the bubble accumulation and growth in the process of landfill gas production, a model of LFG bubble generation in porous media is established. Differentiate the equation of ideal gas law yields

$$\frac{\partial \theta_g}{\partial t}=\frac{RT}{p_g M_g}\frac{\partial m_g}{\partial t}-\frac{m_g RT}{p_g^2 M_g}\frac{\partial p_g}{\partial t} \tag{3}$$

where m_g is the mass of gas per unit volume; R is the ideal gas state constant; T is the gas temperature; p_g is bubble pressure; M_g is the molar mass of the gas.

Introducing the gas production rate $\partial m_\mathrm{g}/\partial t$, the relation between gas and liquid pressures yields the equilibrium equation in terms of LFG bubble pressure as:

$$p_{\mathrm{g}}^{2}\nabla^{2}(p_{\mathrm{g}}-\mathrm{A}p_{\mathrm{g}}^{\frac{1}{3}})=\mathrm{B}\frac{\partial p_{\mathrm{g}}}{\partial t}\text{-C}p_{\mathrm{g}} \tag{4}$$

The coefficients A, B and C are :

$$\mathrm{A}=\frac{2T_{\mathrm{s}}\cos\theta}{\sqrt[3]{\frac{3m_{\mathrm{g}}RT}{4\pi NM_{\mathrm{g}}}}}\text{ , }\mathrm{B}=\frac{\rho_{\mathrm{l}}gm_{\mathrm{g}}RT}{k_{\mathrm{w}}M_{\mathrm{g}}}\text{ ,}\mathrm{C}=\frac{\rho_{\mathrm{l}}gRT}{k_{\mathrm{w}}M_{\mathrm{g}}}\frac{\partial m_{\mathrm{g}}}{\partial t} \tag{5}$$

where T_{s} is the surface tension coefficient; θ is the contact angle; N is the total number of bubbles in a unit volume.

2.1.3 Bubble force equilibrium model

The stress state of LFG bubbles determines the occurrence state and movement form of bubbles. To determine the development stage of bubbles, it is necessary to establish a force balance equation for a single LFG bubble and analyse the force of a single bubble, as shown in Figure 1.

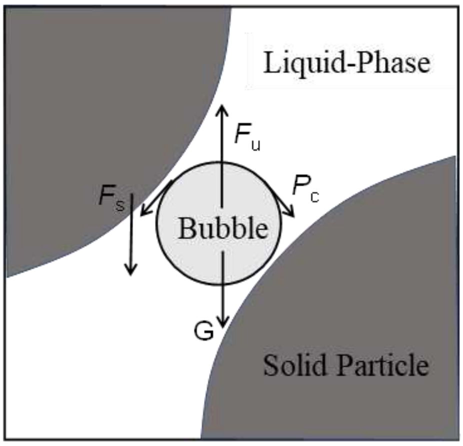

Figure 1. *Force on single bubble*

According to the liquid buoyancy F_{u}, bubble weight G, porous medium resistance F_{s} and capillary pressure P_{c} of a single bubble, the force balance equation of the bubble is established as follows:

$$F_{u}-G-F_{s}(n,u)-P_{c}=(\frac{\partial u_{\mathrm{b}}}{\partial t}+u_{\mathrm{b}}\nabla u_{\mathrm{b}})m_{g} \tag{6}$$

The bubble buoyancy and porous medium resistance can be written as

$$F_{u}=\rho_{l}gV_{g}\text{, }F_{s}(n,u)=A_{\mathrm{s}}[\frac{150\mu_{b}u_{b}(1-n)^{2}}{d_{p}^{2}n^{3}}+\frac{1.75\rho_{g}u_{b}^{2}(1-n)^{2}}{d_{p}n^{3}}]V_{g} \tag{7}$$

where u_{b} is the velocity of the bubble; m_{g} is the mass of the bubble ; A_{s} is the correction factor of liquid film contact surface ; ρ_{1} is the liquid density ; V_{g} is the bubble volume ; ρ_{g} is the gas phase density ; μ_{b} is the dynamic viscosity of gas ; d_{p} is the average particle size of solid particles ; n is the porosity of porous media.

2.2 Two-fluid model in saturated area

LFG bubble generation and liquid-gas migration in the highly saturated region includes two stages. The second stage is the relative migration of liquid-gas after LFG bubble detachment and it can be modelled by a liquid-gas two-fluid model in highly saturated region by introducing porous media resistance condition on the basis of classical Navier-Stokes equation. The liquid-gas two-fluid model in the highly saturated region includes three parts: mass conservation equation and momentum conservation equation, liquid-gas two-phase flow drag model and porous medium resistance model. The volume fraction model is used to describe the discontinuous distribution of leachate and LFG bubbles.

2.2.1 Mass and momentum conservation equation

The mass and momentum conservation equations of the fluid are shown as follows:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = Q \tag{8}$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) + \nabla \cdot \boldsymbol{\tau} = \text{-}\nabla p + \mathbf{S} \tag{9}$$

where $\boldsymbol{\tau}$ is the shear stress tensor, S is the momentum source term, including the liquid-gas two-phase resistance momentum exchange term $S_{\mathrm{i,\,j}}$ and the porous medium momentum loss term S_{Ergun}.

2.2.2 Liquid-gas two-phase resistance momentum exchange term $S_{\mathrm{i,\,j}}$

The liquid-gas two-phase resistance exchange phase $S_{\mathrm{i,\,j}}$ is composed of interphase drag force F_{drag}, lift force F_{lift} and virtual mass force F_{vm}. The equation is as follows:

$$S_{i,j} = n_i (F_{\mathrm{drag}} + F_{\mathrm{lift}} + F_{\mathrm{vm}}) \tag{10}$$

The equations of drag source term, lift source term and virtual mass force source term are as follows:

$$\begin{cases} S_{\mathrm{drag,\,g}} = \dfrac{3}{4}\alpha(n-\alpha)[(n-\alpha)\dfrac{C_{\mathrm{D,l}}\rho_{\mathrm{g}}}{d_{\mathrm{l}}} + \alpha\dfrac{C_{\mathrm{D,g}}\rho_{\mathrm{l}}}{d_{\mathrm{g}}}]|\mathbf{u}_{\mathrm{r}}|\mathbf{u}_{\mathrm{r}} \\ S_{\mathrm{lift,g}} = \alpha(n-\alpha)[(n-\alpha)C_{\mathrm{L,l}}\rho_{\mathrm{g}} + \alpha C_{\mathrm{L,g}}\rho_{\mathrm{l}}]\mathbf{u}_{\mathrm{r}} \times \nabla \times \mathbf{u}_{\mathrm{g}} \\ S_{\mathrm{vm}} = \alpha(n-\alpha)C_{\mathrm{vm}}\rho_{\mathrm{l}}(\dfrac{\mathrm{D}\mathbf{u}_{\mathrm{l}}}{\mathrm{Dt}} \text{-} \dfrac{\mathrm{D}\mathbf{u}_{\mathrm{g}}}{\mathrm{Dt}}) \end{cases} \tag{11}$$

where α is the liquid phase volume fraction ; $C_{\mathrm{D,i}}$ is the drag coefficient ; $C_{\mathrm{L,i}}$ is the lift model coefficient ; C_{vm} is the virtual mass coefficient.

2.2.3 Porous media resistance model

The resistance of porous media is calculated by Ergun resistance model which describes the viscous energy loss of laminar flow and the kinetic energy loss of turbulent flow. The resistance equation of porous media is as follows:

$$\begin{cases} S_{\mathrm{Ergun}} = n_i \cdot F_{\mathrm{s}}(n,u) = K_{\mathrm{Ergun}}\mathbf{u}_{\mathrm{r}} \\ K_{\mathrm{Ergun}} = A[\dfrac{150\mu_i(n-\alpha_i)^2}{\alpha_i d_i^2 n^2} + \dfrac{1.75\rho_i(n-\alpha_i)|\mathbf{u}_{\mathrm{r}}|}{d_i n}] \end{cases} \tag{12}$$

where K_{Ergun} is the fluid-solid resistance.

2.2.4 Volume fraction model

In the liquid-gas two-fluid model in the high saturation region of landfill, the discontinuous distribution area of liquid-gas is described by the volume fraction model, and the phase equation and phase momentum equation with volume fraction as the key variable are established. The spatial distribution mesh of liquid and gas is presented by volume fraction α. When α = 0, the mesh is filled by gas phase. When α = 1, the mesh is filled by liquid phase; when 0 < α < 1, it is the liquid-gas interface mesh. By locating the continuous interface mesh, the liquid-gas interface can be determined, and then the discontinuous distribution of liquid-gas in the whole calculation space can be accurately described. The phase equation of volume fraction α is as follows:

$$\frac{\mathrm{D}\rho}{\mathrm{Dt}} = \frac{\mathrm{D}[\alpha(\rho_{\mathrm{l}} \text{-} \rho_{\mathrm{g}}) + n\rho_{\mathrm{g}}]}{\mathrm{Dt}} = 0 \tag{13}$$

Based on the phase continuity equation of the volume fraction model, the momentum conservation equation of the liquid-gas two-phase flow model is introduced, and the phase momentum equation of the volume fraction model is obtained as follows:

$$\begin{cases}\dfrac{\partial \mathbf{u}_i}{\partial t}+\mathbf{u}_i\cdot\nabla\mathbf{u}_i+\dfrac{\mathbf{u}_iQ_i}{\alpha_i\rho_i}-\nu_{eff,i}\dfrac{\nabla\alpha_i}{\alpha_i}\cdot(\nabla\mathbf{u}_i)+\dfrac{\nabla\alpha_i}{\alpha_i}\cdot\mathbf{R}_{c,i}-\nabla\cdot(\nu_{eff,i}\nabla\mathbf{u}_i)+\nabla\cdot\mathbf{R}_{c,i}\\ =-\dfrac{\nabla p_i}{\rho_i}+\mathrm{g}+\dfrac{\mathbf{S}_{i,j}}{\alpha_i\rho_i}+\dfrac{\mathbf{S}_{Ergun,i}}{\alpha_i\rho_i}\\ \mathbf{R}_{c,i}=-\nu_{eff,i}\nabla\mathbf{u}_i^{\mathrm{T}}+\dfrac{2}{3}\nu_{eff,i}\left(\nabla\cdot\mathbf{u}_i\right)\mathbf{I}+\dfrac{2}{3}\kappa_{i,t}\mathbf{I}\end{cases} \tag{14}$$

where $V_{eff,i}$ is the equivalent fluid viscosity ; ***u*** is the fluid velocity tensor ; Q is the source term ; $\kappa_{i,t}$ is the turbulent kinetic energy of the liquid phase and the gas phase under Reynolds time-average condition.

3 MULTI-FIELD AND MULTI-PHASE COUPLED MODEL FOR AEROBIC LANDFILLS

The up-to-date coupled models for aerobic landfills rarely considered solute transport of carbon and nitrogen elements, and non-equilibrium solid-liquid heat transfer caused by the leachate recirculation. To comprehensively describe the stabilization process of aerobic landfills, based on the existing multi-field and multi-phase cou-pled model for aerobic landfills, further work has been carried out: (1) Methane oxidation, nitrification and denitrification, and aerobic and anaerobic biodegradation in the liquid phase were all considered, allowing the investigation of the migration process of gas components (N_2, O_2, H_2O, CO_2, and CH_4) and leachate solutes (COD, NH_3-N, and NO_3-N); (2) The local thermal non-equilibrium was considered, which is significant in the simulation of leachate recirculation during aeration; (3) the mechanical stress-strain behaviors and the time dependent deformation (i.e., creep-induced and biodeg-radation-induced deformations) were taken into account so that the nonuniform settlement of landfills under aeration can be investigated (Wu et al, 2023).

3.1 Biochemical degradation model

In the biochemical degradation model, in order to further study the flow of carbon C and nitrogen N in the solid-liquid-gas three-phase waste during the degradation process, methane oxidation (⑤), nitrification and denitrification reactions (⑧, ⑨) and aerobic and anaerobic biodegradation in the liquid phase (③, ④) are added to the existing models. The reactions are shown in Figure 2.

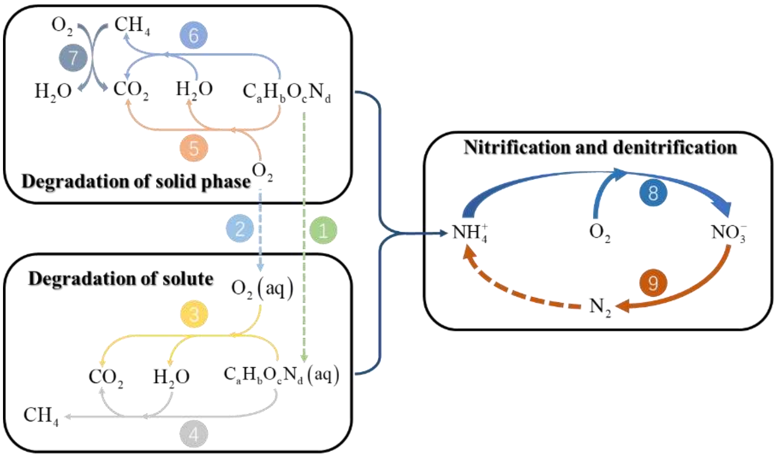

Figure 2. *Biodegradation reaction process in landfills under aeration*

3.1.1 Methane oxidation equation

There exists methane oxidation reaction among gas components in aerobic landfills, that is, methane is oxidized into carbon dioxide and water vapor under the action of methane bacteria, and heat is released. The flow process of C in the gas phase is supplemented by the consideration of methane oxidation, and the equation is as follows:

$$\begin{gathered}\mathrm{CH_4{+}2O_2 \rightarrow CO_2{+}2H_2O} \\ \Delta H_3 = -55668\frac{\mathrm{kJ}}{\mathrm{kg\ CH_4}}\end{gathered} \tag{15}$$

3.1.2 Nitrification and denitrification equations

Nitrification is the conversion of ammonia to nitrite or nitrate by nitrifying bacteria under aerobic conditions, while denitrification is the conversion of nitrate to nitrogen or nitrous oxide under aerobic conditions. To simplify the nitrification and denitrification reaction, it was assumed that the only product of the nitrification reaction is nitrate, and the only product of the denitrification reaction is nitrogen. The N flow during the accelerated stabilization process of aerobic landfill can be studied by adding nitrification and denitrification reactions in the biochemical degradation module. The nitrification and denitrification reactions are as follows:

$$\mathrm{NH_3{+}2O_2 \rightarrow HNO_3 + H_2O} \quad , \quad \Delta H_4 = -21176\frac{\mathrm{kJ}}{\mathrm{kg\ NH_3}} \tag{16}$$

$$\mathrm{2NO_3^- + 12H^+ + 10e^- \rightarrow N_2 + 6H_2O} \quad , \qquad \Delta H_5 = 741\frac{\mathrm{kJ}}{\mathrm{kg\ NO_3^-}} \tag{17}$$

3.1.3 Aerobic and anaerobic biodegradation equations

According to the oxygen concentrations in waste, two biodegradation modes will occur in landfills: aerobic biodegradation and anaerobic biodegradation. The reaction equations for the biodegradation of the degradable organic matter are as follows :

$$\mathrm{C}_a\mathrm{H}_b\mathrm{O}_c\mathrm{N}_d + \frac{b-3d+4a-2c}{4}\mathrm{O_2} \xrightarrow{\text{Biomass}} a\mathrm{CO_2} + \frac{b-3d}{2}\mathrm{H_2O} + d\mathrm{NH_3}, \quad \Delta H_1 = -17360\frac{\mathrm{kJ}}{\mathrm{kg\ C}_a\mathrm{H}_b\mathrm{O}_c\mathrm{N}_d} \tag{18}$$

$$\begin{gathered}\mathrm{C}_a\mathrm{H}_b\mathrm{O}_c\mathrm{N}_d + \frac{4a-b-2c+3d}{4}\mathrm{H_2O} \xrightarrow{\text{Biomass}} \frac{4a-b+2c+3d}{8}\mathrm{CO_2} + \frac{4a+b-2c-3d}{8}\mathrm{CH_4} + d\mathrm{NH_3}, \\ \Delta H_2 = -1672\frac{\mathrm{kJ}}{\mathrm{kg\ C}_a\mathrm{H}_b\mathrm{O}_c\mathrm{N}_d}\end{gathered} \tag{19}$$

where $C_aH_bO_cN_d$ is the molecular formula representing the chemical composition of waste; and a, b, c, and d are the constants representing the contents of carbon, hydrogen, oxygen, and nitrogen.

3.2 Non-equilibrium solid-liquid heat transfer and time dependent deformation

Leachate recirculation is usually used to decrease the elevated temperatures within landfills after aeration. In this scenario, the general local equilibrium heat transfer equation will no longer be applicable as the three phases in waste are not isothermal. The local non-equilibrium heat transfer equation takes the solid phase and the gas phase as the isothermal state, while the liquid phase is described by a separate temperature variable, which can effectively simulate the recirculation condition. The heat exchange between liquid and solid can be calculated using the heat transfer coefficient. However, there are few researches on the thermal properties of waste, so the heat transfer coefficient of waste can be derived based the assumption of sphere and uniform waste particles as follows:

$$\begin{cases} h_{\mathrm{ws}} = \dfrac{\left(2.0 + 1.1\mathrm{Pr}^{1/3}\,\mathrm{Re}^{0.6}\right)\cdot\Gamma_{\mathrm{w}}}{L} \\ L = \dfrac{d}{2}\sqrt{\dfrac{\pi}{1-n}}, \mathrm{Re} = \dfrac{\rho_{\mathrm{w}}\left|\mathbf{v}_{\mathrm{wr}}\right| L}{\mu_{\mathrm{w}}}, \mathrm{Pr} = \dfrac{\mu_{\mathrm{w}} H_{\mathrm{w}}}{\Gamma_{\mathrm{w}}} \end{cases} \tag{20}$$

where h_{ws} is the convective heat transfer rate ; L is the characteristic length of solid particles ; Γ_{w} is the thermal conductivity of liquid phase ; R_{e} is Reynolds number ; P_{r} is the Prandtl number ; d is the characteristic length of the circulation channel ; V_{wr} is the velocity of fluid ; ρ_{w} is the fluid density ; μ_{w} is the hydrodynamic viscosity ; H_{w} is the specific heat capacity of fluid.

Nonuniform settlement will occur in aerobic landfills due to uneven distributions of oxygen and biodegradation degree. The nonuniform settlement may threaten the embedded pipelines. To describe this nonuniform settlement more accurately, it is necessary to introduce the deformation caused by aerobic biodegradation and creep, which can be calculated by the following formula :

$$\mathrm{d}\varepsilon_{\mathrm{bc}} = \frac{\left(1+\Lambda\right)}{\left(1+\varepsilon_{\mathrm{V}}\right)V_0}\frac{\mathrm{d}m}{\rho_{\mathrm{s}}} + C_{\mathrm{c}}C_{\mathrm{b}}\Delta\sigma' e^{-C_{\mathrm{c}}t}\mathrm{d}t \tag{21}$$

where Λ is a dimensionless factor ; V_0 is the initial volume of waste ; ε_V is the volumetric strain; C_{c} and C_{b} are the rate constants of creep ; $\Delta\sigma'$ is the change in the average effective stress.

4 CONCLUSIONS

In order to describe the discontinuous flow of leachate-gas below leachate level and the three-phase stabilization process of aerobic landfill, this study first established a leachate-gas migration model considering LFG bubble formation, accumulation and two-fluid flow in highly saturated area. This model mainly consisted of bubble generation model and liquid-gas two-fluid model. The former one included liquid phase continuity equation, LFG bubble generation model in porous medium and bubble force equilibrium equation. After LFG bubble detachment, the liquid-gas two-fluid model was established by introducing the porous medium resistance condition based on the classical Navier-Stokes equation.

Secondly, new sub-models of methane oxidation, nitrification and denitrification, solute transports, non-equilibrium solid-liquid heat transfer, and biodegradation-induced and creep deformation are added to the existing aerobic landfill multi-field coupled models. This model can be used to study the accelerated stabilization of landfilled waste from solid, gas and liquid phases, and the flows of carbon and nitrogen elements among different phases and components under aeration.

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