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## A biochemical-thermo-hydro-mechanical coupling of degradable soils

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### ABSTRACT

A general framework of coupled biochemical-thermo-hydro-mechanical (THMBC) processes has been developed to analyze the complex phenomena in degradable soils, such as municipal solid and natural gas hydrate, whose solid skeleton can be decomposed by biological or chemical reactions. The frame contains the linear momentum equilibrium equation, the mass conservation equations for the liquid and gas phases, the energy conservation equation. The evaporation and condensation of water, and the dissolution of gas in water are considered in the mass conservation equation of the fluid. The biochemical reaction rate can be used to link the source and sink terms of the fluid with solid mass loss, meanwhile to give a quantitative description of changes in porosity and strain. The impact of the solid mass loss and the porosity change on the hydro-mechanical properties are involved. As a case study, a model describing the coupling process of landfilled MSW was proposed. In this model, the constitutive model considering the influence of degradation was used, and the degradation chemical formula of the degradable component was given. The results of CAR1 experiment were compared with numerical simulations.

**Keywords:** biochemical-thermo-hydro-mechanical coupling, degradable soils, numerical modelling

## 1 INTRODUCTION

Degradable soils are those which have a solid skeleton that can be converted into liquid or gas phases by biological and chemical processes with mass loss and changes of the grain size.

Four kinds of fluid exist in degradable soils. They are pore water, dissolved air, undissolved air and vapor. The former two are counted as pore liquids, while the latter two are pore gases. Different scripts are used to distinguish them.  $w$  for pore water,  $da$  for dissolved air,  $ua$  for undissolved air and  $v$  for vapor.

Superscripts are for apparent densities in REV while subscripts are for real densities. The relationship between apparent and real densities are  $\rho^w = \phi S_w \rho_w$ ,  $\rho^v = (1 - S_w) \phi \rho_v$ ,  $\rho^{ua} = (1 - S_w) \phi \rho_{ua}$ , and  $\rho^{da} = \phi S_w c_{da}$ . where  $\phi$  is porosity,  $S_w$  is saturation,  $c_{da}(\text{kg} \cdot \text{m}^{-3})$  is the mass concentration of dissolved air in solute.

Governing equations for all constituents have a similar form as

$$\frac{\partial \rho^\pi}{\partial t} + \nabla \cdot J_\pi = Q_\pi \quad (1)$$

where  $J_\pi(\text{kg} \cdot \text{m}^{-2} \cdot \text{s}^{-1})$  and  $Q_\pi(\text{kg} \cdot \text{m}^{-3} \cdot \text{s}^{-1})$  are the mass flux and source term of substance  $\pi$ ,

respectively.

In this study, a general framework of coupled biochemical-thermo-hydro-mechanical (THMBC) processes has been developed to analyze the complex phenomena in degradable soils, such as municipal solid and natural gas hydrate, whose solid skeleton can be decomposed by biological or chemical reactions.

## 2 CONSTITUTIVE EQUATIONS

### 2.1 Biochemical reaction

According to the principle of mass conservation, the total mass of reactant and the product in the  $j$  th biochemical reaction are the same, and this can be expressed in the following form

$$C_{j,i} \cdot S_i = 0 \quad (2)$$

where  $C_{j,i}$  is the mass ration coefficient,  $j$  and  $i$  stand for the number of biochemical reaction and compound, respectively.  $S_i(\text{kg} \cdot \text{m}^{-3})$  is the mass concentration of the  $i$  th substance.

Generally, the mass changing rate of each compound can be expressed as follows

$$\frac{dS_i}{dt} = \alpha_i \sum (C_{j,i} R_j) \quad (3)$$

where  $\alpha_i$  is the dimensionless transfer coefficient for  $S_i$ , defined as  $1/\theta$  ( $\theta$  is the volumetric ratio of water) for solutes and equal to 1 for other compound,  $R_j$  is the reaction rate ( $\text{kg} \cdot \text{m}^{-3} \cdot \text{s}^{-1}$ ).

Consider there are  $w$  kinds of solid compounds,  $x$  kinds of solution,  $y$  kinds of gas compounds in the degradable soil, and  $z$  stands for water, the source terms for solid, gas, water and solute could be expressed as

$$Q_s = \sum_1^w \frac{dS_i}{dt}, \quad Q_a = \sum_{w+x+1}^{w+x+y} \frac{dS_i}{dt}, \quad Q_w = \frac{dS_z}{dt}, \quad \text{and}$$

$$Q_{s_i} = \frac{dS_i}{dt} \quad (w+1 \leq i \leq w+x).$$

If intra-particle water release exists, there should be a special mass change item for it, with  $z$  standing for intra-particle water.

$$Q_{sw} = \frac{dS_z}{dt} \quad (4)$$

It should be noticed that the intra-particle water belongs to solid phase before release, while it belongs to liquid phase afterwards.

## 2.2 Deformation

The total strain  $\varepsilon$  due to stress and biochemical reaction can be written as a function of effective stress and current solid mass, and can be expressed as:

$$\varepsilon = f(\boldsymbol{\sigma}', M_{sd}), \quad M_{sd} = \sum_1^w S_i \quad (5)$$

## 2.3 Porosity

Based on Zienkiewicz's theory of effect of hydrostatic pressure on the deformable solids, constitutive equation for porosity  $\phi$  considering thermal deformation, mechanical deformation, solid mass change and intra-particle water release is

$$\frac{\partial \phi}{\partial t} = (\alpha - \phi) \nabla \cdot \mathbf{v}_s + \frac{\alpha - \phi}{K_s} \cdot \frac{\partial p_s}{\partial t} - \beta_s (\alpha - \phi) \frac{\partial T}{\partial t} - \phi \frac{Q_s}{\rho_s} - \frac{Q_{sw}}{\rho_w} \quad (6)$$

where  $\alpha$  is Biot coefficient,  $\mathbf{v}_s$  ( $\text{m} \cdot \text{s}^{-1}$ ) is velocity of solid phase,  $K_s$  (Pa) is bulk modulus of solid grain,  $p_s$  (Pa) is average pore pressure (Zienkiewicz et al., 1985).

## 2.4 Gas State Equation

The equations of state of a perfect gas, applied to dry air, vapor and the gas mixture are

$$p_{ua} = \rho_{ua} RT / M_a, \quad p_v = \rho_v RT / M_w \quad (7)$$

$$p_g = p_{ua} + p_v, \quad \rho_g = \rho_{ua} + \rho_v \quad (8)$$

$$M_g = \left( \frac{\rho_v}{\rho_g} \cdot \frac{1}{M_w} + \frac{\rho_{ua}}{\rho_g} \cdot \frac{1}{M_a} \right)^{-1} \quad (9)$$

Eq.(8) expresses the Dalton's law, and where  $p_\pi$  (Pa),  $\rho_\pi$  ( $\text{kg} \cdot \text{m}^{-3}$ ) and  $M_\pi$  are pressure, density and molar mass of substance  $\pi$ , respectively.  $T$  (K) is temperature.

The vapor pressure  $p_v$  can be obtained from the Kelvin-Laplace equation:

$$p_v = p_{vs} \exp\left(\frac{p_c M_w}{\rho_w RT}\right) \quad (10)$$

where saturated vapor pressure  $p_{vs}$  is a function of temperature.

## 2.5 Air Dissolving

The specific mole fraction of the gas dissolved in the pore water  $x_{da}$  is equal to  $X_{da}/(X_{da} + X_w)$ , where  $X_{da}$  (mol) and  $X_w$  (mol) are amount of substance of solute and solvent, respectively. The relationship of  $x_{da}$  and  $c_{da}$  has the form as:

$$c_{da} = \rho_w \frac{x_{da} M_a}{1 - x_{da} M_w} \quad (11)$$

## 2.6 Transport of Fluid

For pore-liquid, Darcy's law is used to describe the convention of pore water and the dissolved air.

$$J_{cw} = \rho_w \frac{\mathbf{k}k_{rl}}{\mu_l} (-\nabla p_g + \nabla p_c + \rho_w \mathbf{g}) \quad (12)$$

$$J_{cda} = c_{da} \frac{\mathbf{k}k_{rl}}{\mu_l} (-\nabla p_g + \nabla p_c + \rho_w \mathbf{g}) \quad (13)$$

For pore gas, the convention part for vapor and undissolved air are described as:

$$J_{cv} = \rho_v \frac{\mathbf{k}k_{rg}}{\mu_g} (-\nabla p_g + \rho_g \mathbf{g}) \quad (14)$$

$$J_{cua} = \rho_{ua} \frac{\mathbf{k}k_{rg}}{\mu_g} (-\nabla p_g + \rho_g \mathbf{g}) \quad (15)$$

Diffusive-dispersive flux is governed by Fick's law.

$$J_g^v = D_g^v \nabla \rho_v, \quad J_g^{ua} = D_g^{ua} \nabla \rho_{ua} \quad (16)$$

The total flux of water (liquid water and vapor) and air (dissolved and undissolved) are:

$$J_w = J_{cw} + J_{cv} + J_g^v = \rho_w \frac{\mathbf{k}k_{rl}}{\mu_l} (-\nabla p_g + \nabla p_c + \rho_w \mathbf{g}) + \rho_v \frac{\mathbf{k}k_{rg}}{\mu_g} (-\nabla p_g + \rho_g \mathbf{g}) + \rho_g D_g \nabla \left( \frac{\rho_v}{\rho_g} \right) \quad (17)$$

$$J_a = J_{cda} + J_{cua} + J_g^{ua} = c_{da} \frac{\mathbf{k}k_{rl}}{\mu_l} (-\nabla p_g + \nabla p_c + \rho_w \mathbf{g}) + \rho_{ua} \frac{\mathbf{k}k_{rg}}{\mu_g} (-\nabla p_g + \rho_g \mathbf{g}) + \rho_g D_g \nabla \left( \frac{\rho_{ua}}{\rho_g} \right) \quad (18)$$

### 2.7 Permeability and Saturation

The intrinsic permeabilities for liquid and gas is assumed to be identical. Laboratory water permeability and air permeability tests were carried out to study the intrinsic and relative permeabilities of MSW at different depths (Xu et al., 2014). A modified intrinsic permeability model is introduced, and the variation of the intrinsic permeability  $\mathbf{k}$  ( $\text{m}^2$ ) is related to the porosity.

$$\mathbf{k} = \mathbf{k}_0 \exp \left( A \left( \frac{\phi}{\phi_0} - 1 \right) \right) \quad (19)$$

where  $\mathbf{k}_0$  ( $\text{m}^2$ ) is the referent intrinsic permeability with the referent porosity  $\phi_0$ .  $A$  is a fitted model parameter for the measurement of in-situ samples from different depths and ages.

The capillary pressure  $p_c$  and relative permeability  $k_{r\pi}$  ( $\text{m} \cdot \text{s}^{-1}$ ) is related to effective water saturation  $S_{eff}$  following the vG-M model.

$$k_{rl} = S_{eff}^{0.5} \left[ 1 - \left( 1 - S_{eff}^{1/m_v} \right)^{m_v} \right]^2 \quad (20)$$

$$k_{rg} = \left( 1 - S_{eff} \right)^{0.5} \left( 1 - S_{eff}^{1/m_v} \right)^{2m_v} \quad (21)$$

$$p_c = \frac{1}{\alpha_v} \left( S_{eff}^{(n_v-1)/n_v} - 1 \right)^{1/n_v} \quad (22)$$

where  $\alpha_v$ ,  $m_v$ ,  $n_v$  are parameters in the vG-M model, and effective water saturation  $S_{eff}$  can be expressed as:

$$S_{eff} = \frac{S_w - S_{wr}}{S_{wmax} - S_{wr}} \quad (23)$$

where  $S_{wr}$  is the residual water saturation,  $S_{wmax}$  is the maximum water saturation.

### 2.8 Evaporation and condensation

$\dot{m}_{vap}$  ( $\text{kg} \cdot \text{m}^{-3} \cdot \text{s}^{-1}$ ) and  $\Delta H_{vap}$  ( $\text{J} \cdot \text{kg}^{-1}$ ) are phase change rate and enthalpy of evaporation, respectively. For condensation the values are negative.

## 3 MACROSCOPIC BALANCE EQUATIONS

Use capillary pressure  $p_c$ , total gas pressure  $p_g$  and temperature  $T$  as primary variables to build a system of partial derivative equations.

### 3.1 Linear momentum balance equations

The linear momentum balance equations of the mixture in terms of total Cauchy stress  $\boldsymbol{\sigma}$  (Pa) assumes the form as:

$$\nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{g} = 0 \quad (24)$$

Where the density of the mixture  $\rho$  is equal to  $[(1 - \phi)\rho_s + \phi S_w \rho_w + \phi(1 - S_w)\rho_g]$ , the total stress  $\boldsymbol{\sigma}$  is equal to  $(\boldsymbol{\sigma}' - \alpha p_s \mathbf{I})$  (Fredlund et al., 1993), in which the Biot coefficient  $\alpha$  is equal to  $(1 - K_D/K_S)$  (Sanavia et al., 2005).  $K_D$  (Pa) is the bulk moduli of soil. The average pore pressure  $p_s$  (Pa) is calculated using Bishop coefficient  $\chi$ , and can be expressed as:

$$p_s = p_g - \chi p_w \quad (25)$$

### 3.2 Mass balance equations

For water

$$\begin{aligned} & \left[ S_w \rho_w + \rho_v (1 - S_w) \right] \frac{\partial \phi}{\partial t} + \phi (\rho_w - \rho_v) \frac{\partial S_w}{\partial t} \\ & + \phi (1 - S_w) \frac{\partial \rho_v}{\partial t} + \nabla \cdot \left[ \rho_g D_g \nabla \left( \frac{\rho_v}{\rho_g} \right) \right] \\ & + \nabla \cdot \left[ \rho_w \frac{\mathbf{k}k_{rl}}{\mu_l} (-\nabla p_g + \nabla p_c + \rho_w \mathbf{g}) \right] \\ & + \nabla \cdot \left[ \rho_v \frac{\mathbf{k}k_{rg}}{\mu_g} (-\nabla p_g + \rho_g \mathbf{g}) \right] = Q_w - Q_{sw} \end{aligned} \quad (26)$$

For gas

$$\begin{aligned} & \phi (1 - S_w) \frac{\partial \rho_a}{\partial t} + [S_w c_a + (1 - S_w) \rho_a] \frac{\partial \phi}{\partial t} \\ & + (\phi c_a - \phi \rho_a) \frac{\partial S_w}{\partial t} + \phi S_w \frac{\partial c_a}{\partial t} + \nabla \cdot \left[ \rho_g D_g \nabla \left( \frac{\rho_a}{\rho_g} \right) \right] \\ & + \nabla \cdot \left[ c_a \frac{\mathbf{k}k_{rl}}{\mu_l} (-\nabla p_g + \nabla p_c + \rho_w \mathbf{g}) \right] \\ & + \nabla \cdot \left[ \rho_a \frac{\mathbf{k}k_{rg}}{\mu_g} (-\nabla p_g + \rho_g \mathbf{g}) \right] = Q_a \end{aligned} \quad (27)$$

### 3.2 Energy balance equation

The energy balance equation of the mixture is

$$\begin{aligned}
& (\rho C_p)_{eff} \frac{\partial T}{\partial t} + J_w C_p^w \cdot \nabla T \\
& + J_a C_p^g \cdot \nabla T - \nabla \cdot (\chi_{eff} \nabla T) \\
& = (Q_s C_p^s + Q_w C_p^w + Q_a C_p^g) T - i
\end{aligned} \quad (28)$$

where effective thermal capacity of degradable soil  $(\rho C_p)_{eff}$  ( $J \cdot m^{-3} \cdot K^{-1}$ ) is equal to  $(\rho_s C_p^s + \rho_w C_p^w + \rho_g C_p^g)$ , and effective thermal conductivity of the degradable soil  $\chi_{eff}$  ( $W \cdot m^{-1} \cdot K^{-1}$ ) is equal to  $(\chi_s + \chi_w + \chi_g)$ ,  $C_p^s$  ( $J \cdot kg^{-1} \cdot K^{-1}$ ) and  $\chi_\pi$  is the specific heat capacity and thermal conductivity of substance  $\pi$ , respectively.

Item  $\dot{m}_{vap} \Delta H_{vap}$  considers the contribution of the evaporation and condensation. This balance equation takes into account the heat transfers through conduction and convection as well as latent heat transfer (Lewis et al., 1998) and neglects the terms related to the mechanical work induced by density variations due to temperature changes of the phases and induced by volume fraction changes.

### 3.3 Dissolved solute distribution equation

The dissolved solute transport can be described by the mass conservation equation in the form as:

$$\frac{\partial S_i}{\partial t} + \mathbf{v}^w \nabla S_i - \mathbf{D}_l \nabla^2 S_i = Q_{S_i} \quad (29)$$

The velocity of water  $\mathbf{v}_w$  ( $m \cdot s^{-1}$ ) is described using the Darcy's law:

$$\mathbf{v}_w = \frac{\mathbf{k} k_{rl}}{\mu_w} (-\nabla p_g + \nabla p_c + \rho_w \mathbf{g}) \quad (30)$$

### 3.4 Multicomponent gas distribution equation

Similar to the dissolved solute, gases (such as  $CO_2$ ,  $H_2S$ ,  $CH_4$ ,  $H_2$ ) transport in dry air mixture can be expressed as:

$$\frac{\partial S_i}{\partial t} + \mathbf{v}^g \nabla S_i - \mathbf{D}_g \nabla^2 S_i = Q_{S_i} \quad (31)$$

The velocity of gas  $\mathbf{v}_g$  ( $m \cdot s^{-1}$ ) is described using the Darcy's law:

$$\mathbf{v}_g = \frac{\mathbf{k} k_{rg}}{\mu_g} (-\nabla p_g + \rho_g \mathbf{g}) \quad (32)$$

## 4 CASE STUDY

A case was studied to testify the validation of the model. The model set up was based on the CAR1 experiment done by Beaven (Beaven et al., 2008). In the experiment, 27 kg dry weight of shredded MSW was contained in a cylindrical reactor which had an internal diameter of 480 mm. 90 L leachate saturated and

recirculated through the sample. A constant load was applied to the top boundary. The initial conditions, boundary conditions and source terms are shown in Fig. 1. Full details were given in Beaven et al. 2008.

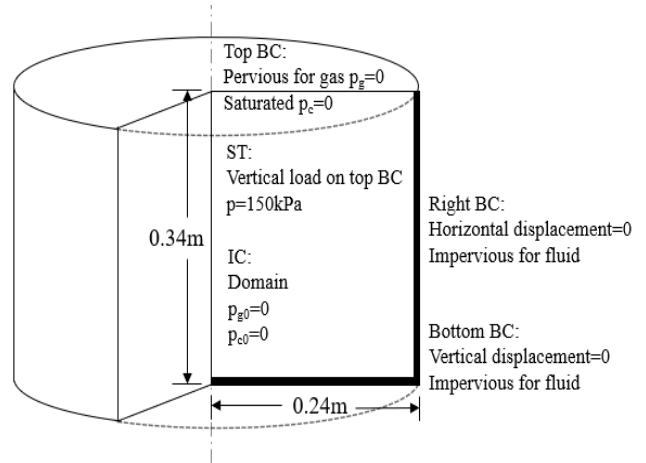
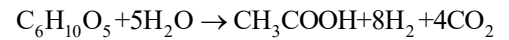


Fig. 1. Model of the reactor

According to the anaerobic two-stage degradation model, hydrolysis and methanogenesis are involved in biochemical process.

Biochemical reactions are listed and numbered from 1 to 7 for subscript  $j$  (Chen et al., 2020)

(1) Fast cellulose hydrolysis:



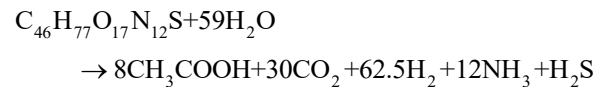
(2) Slow cellulose hydrolysis:



(3) Glucose hydrolysis:



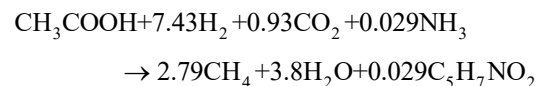
(4) Protein hydrolysis:



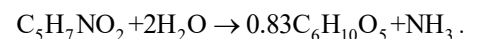
(5) Fat hydrolysis:



(6) Methanogenesis of VFA:



(7) Decay of MB:



Compound are numbered from 1 to 12 for subscript  $i$  in Table 2, the initial weights are also listed.

Table 2. Compound correspondence and initial concentration.

<i>i</i>	1	2	3	4	5	6
Compound	Fast cellulose	Slow cellulose	Glucose	protein	Fat	VFA
Initial Concentration (kg/m <sup>3</sup> )	54.92	83.42	2.89	1.99	1.99	0
<i>i</i>	7	8	9	10	11	12
Compound	MB	H <sub>2</sub> O	CO <sub>2</sub>	H <sub>2</sub> S	CH <sub>4</sub>	H <sub>2</sub>
Initial Concentration (kg/m <sup>3</sup> )	0.1	610	0	0	0	0

Reaction rate for hydrolysis processes is (EL-Fadel et al., 1996)

$$R_j = -k_{Hj} f_w f_{Ih} S_j \quad (j = 1, 2, 3, 4, 5) \quad (33)$$

where  $k_{Hj}$  (d<sup>-1</sup>) is the hydrolysis constant factor,  $f_w$  is the water content dependent coefficient, and  $f_{Ih}$  is the VFA inhibition factor.  $f_w$  and  $f_{Ih}$  have the following formulations, where  $\theta_{\min}$  and  $\theta_{\max}$  are the minimum and maximum water content (kg · m<sup>-3</sup>), respectively.  $K_h$  (kg · m<sup>-3</sup>) and  $n_h$  are the hydrolysis inhibition constant and hydrolysis inhibition exponent, respectively.

$$f_w(\theta) = \frac{\theta - \theta_{\min}}{\theta_{\max} - \theta_{\min}} \quad (34)$$

$$f_{Ih} = \frac{1}{1 + (S_6 / K_h)^{n_h}} \quad (35)$$

Reaction rate for methanogenesis is

$$R_6 = \frac{\theta}{Y} \cdot \frac{k_{m \max} S_7}{k_s + S_6} f_{Im} S_6 \quad (36)$$

where  $Y$  is the ratio of the mass of the increased methanogen to the mass of the substrate VFA consumed.  $k_{m \max}$  (d<sup>-1</sup>) is the maximum growth rate of MB,  $k_s$  (kg · m<sup>-3</sup>) is the half saturation constant of MB,  $f_{Im}$  is the function for the VFA inhibition of MB growth with the following formulation.  $K_m$  (kg · m<sup>-3</sup>) and  $n_m$  are the methanogenesis inhibition constant and the methanogenesis inhibition exponent, respectively.

$$f_{Im} = \frac{1}{1 + (S_6 / K_m)^{n_m}} \quad (37)$$

Reaction rate for MB decay

$$R_7 = \theta k_d S_7 \quad (38)$$

where  $k_d$  (d<sup>-1</sup>) is the decay rate of MB.

Biot coefficient is 1, and bishop coefficient is equal to water saturation, other parameters of coupling model are listed in Table 3.

Table 3. Parameters of coupling model

$k_{H1}$	$k_{H2}$	$k_{H3}$	$k_{H4}$	$k_{H5}$	$\theta_{\min}$	$\theta_{\max}$
0.021	0.0013	0.021	0.021	0.021	0%	85%
$K_h$	$n_h$	$Y$	$k_{m \max}$	$k_s$	$K_m$	$n_m$
12	8	0.1	0.15	2	12	6
$k_d$	$K_D$	$\phi_0$	$\mathbf{k}$	$\alpha_v$	$n_v$	$D_0$
0.0055	32000	0.61	10 <sup>-10</sup>	0.88	1.58	10 <sup>-5</sup>

The comparison between the settlement calculated and measured in the laboratory is given in Fig. 2. It shows that the settlement calculated by the model is slightly smaller than the actual one, perhaps because mechanical creep is not considered.

The comparison between the VFA concentration calculated and measured in the laboratory is given in Fig. 3. It shows the same peak concentration of VFA, but the modelled one declines more slowly after the peak.

The comparison between the cumulative gas production calculated and measured in the laboratory is given in Fig. 4. It shows that the two are very close at first 500 days.

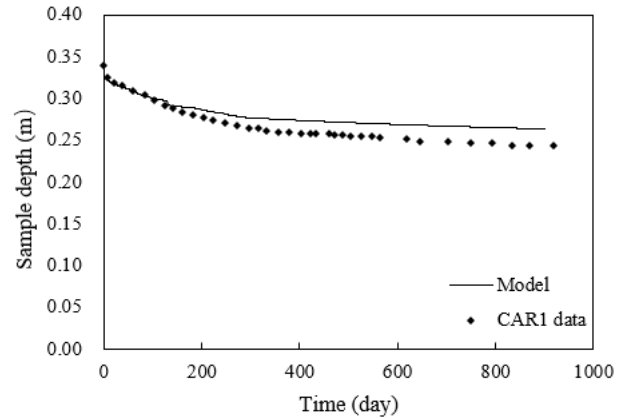


Fig. 2. Modelled settlement compared with CAR1 data.

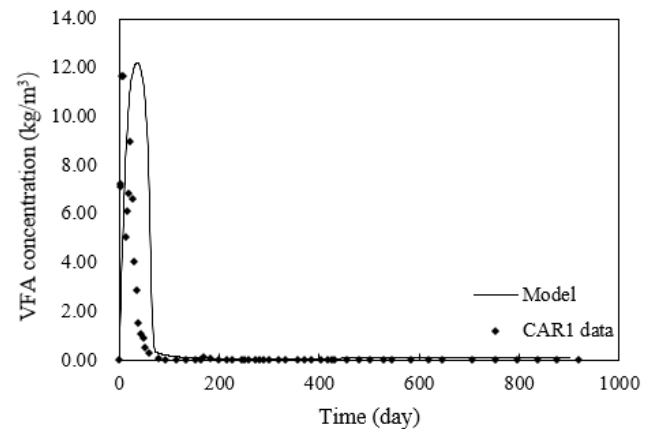


Fig. 3. Modelled VFA concentration compared with CAR1 data.

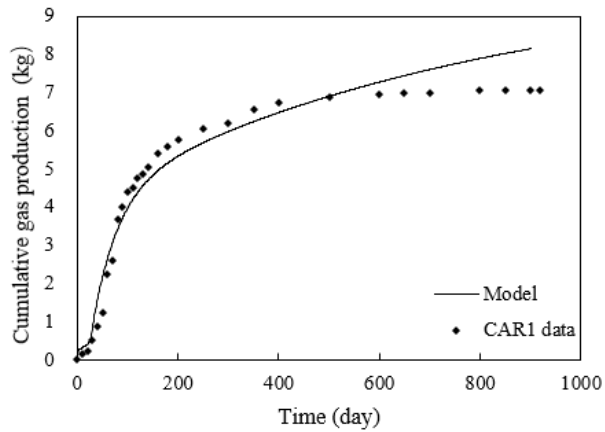


Fig. 4. Modelled cumulative gas production compared with CAR1 data.

## 6 CONCLUSIONS

A framework for biochemical-thermo-hydro-mechanical processes has been developed. This model considered (1) the multi-physics process, including solid skeleton deformation, pore water flow, solute transport, pore gas flow, evaporation and condensation, air dissolving, temperature change and biochemical degradation, (2) the biological degradation induced solid mass transformation of solids, liquids, gases, and solutes.

In addition to MSW problems, the model could also be used to analyze problems such as methane hydration extraction and coal pyrolysis.

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