Modelling of effects of water vapor and temperature gradient on moisture and gas transfer in unsaturated landfill cover

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ABSTRACT

Methane emissions through landfill cover is a complicated multi-physics coupled process, including water-gas-heat transfer and microbial aerobic methane oxidation (MAMO). Due to the relatively high water content of municipal wastes in China, landfill gas generally contains a substantial amount of water vapor. Moreover, the biochemical decomposition of wastes underneath landfill cover results in noticeable temperature gradient across the cover. Nevertheless, effects of water vapor and temperature gradient on water and gas distributions in landfill cover are not clear. A new theoretical model of water-gas-heat reactive transfer and MAMO in unsaturated soils was developed by incorporating effects of vapor flow and temperature gradient on water and gas transfer. The newly proposed model was implemented in a finite-element software COMSOL. The model was verified by (i) a published soil column test simulating MAMO; and (ii) a soil column test subject to heating. The model is capable of describing liquid water-vapor transfer, multi-component gas transfer (e.g., CH4, CO2, N2 and O2), heat transfer and MAMO. The theoretical model and the related numerical code could serve as a useful tool for landfill cover design for mitigating methane emissions.

Keywords: coupled process, vapor, temperature gradient, landfill cover, methane oxidation

1 INTRODUCTION

Methane emissions from municipal landfill pose a risk to the public as an explosive gas and to the climate as a strong greenhouse gas. The transfer of methane through landfill cover involves water-gas-heat coupled process as well as microbial aerobic methane oxidation (MAMO), which consumes methane by methanotrophs. MAMO is significantly affected by soil moisture and temperature.

In China, landfill gas contains substantial amount of vapor due to water generation by decomposition of high organic content of municipal wastes. The relative humidity of landfill gas could reach almost 100% (Li et al., 2018). It is well recognized that the condensation and evaporation can alter soil moisture distribution, which affects both water-gas-heat transfer as well as MAMO. Moreover, heat generation by decomposition of decomposed wastes can result in a temperature gradient along landfill cover. A noticeable temperature difference of up to 30 °C was recorded in an in-situ monitor of landfill cover of thickness of 0.9 m in Xi’an, China (Zhan et al., 2020). Temperature gradient in the landfill cover not only affects the activity of methanotrophs, but also affects the migration of moisture and gas. However, effects of vapor and temperature gradient on moisture and gas transfer in landfill cover are not clear.

Various theoretical models considering water-gas-heat coupled process have been proposed to depict methane transfer through landfill cover (Garg and Achari, 2010; Feng et al., 2017). The theoretical model proposed by Ng et al. (2015) is relatively advanced, which is capable of describing liquid water-vapor transfer, multi-component gas transfer (e.g., CH4, CO2, N2 and O2), heat transfer and MAMO. The theoretical model and the related numerical code could serve as a useful tool for landfill cover design for mitigating methane emissions.

2 THEORETICAL MODEL DEVELOPMENT

The reference model proposed by Ng et al. (2015) is further developed by including (i) vapor flow; and (ii) water and gas flow driven by temperature-gradient. The following assumptions are made: (i) soil skeleton is rigid; (ii) ideal gas law is valid; (iii) thermal equilibrium state is reached for soil particle, gas and water; and (iv) equilibrium state is reached for liquid water and vapor. The governing equations are given as follows.

2.1 Moisture flow in soil

Moisture flow in soil consists of both liquid water
flow and vapor flow. According to water mass balance, the liquid water flow could be depicted as follows (Ng et al., 2015):

$$
\frac{\partial (\rho_l \theta)}{\partial t} = -\nabla (\rho_l v_l) + \rho_r M_{H,O} R_l - \Gamma_v
$$

(1)

where $\rho_l$ is liquid water density (kg/m$^3$); $\theta_l$ is volumetric water content (dimensionless); $t$ is time (s); $v_l$ is liquid water flow velocity (m/s); $\rho_r$ is dry soil density (kg/m$^3$); $M_{H,O}$ is the molar mass of water (0.018 kg/mol); $R_l$ is water generation rate by MAMO per unit mass of dry soil (mol kg$^{-1}$ dry soil s$^{-1}$); and $\Gamma_v$ is the evaporation rate (kg/s). The physical meaning of Eq. (1) is that the change in mass of liquid water is caused by the net inflow of liquid water ($-\nabla (\rho_l v_l)$), water generation by MAMO ($\rho_r M_{H,O} R_l$), and water evaporation ($\Gamma_v$).

$v_l$ is determined using the Darcy’s law:

$$
v_l = k_{rw} \frac{k_l}{u_l} (\nabla P_w + \gamma v \nabla z)
$$

(2)

where $k_{rw}$ is the relative water permeability (dimensionless); $k_l$ is the intrinsic permeability of soil (m$^2$); $u_l$ is the liquid water viscosity (Pa s); $P_w$ is pore-water pressure (Pa); $\gamma$ is the unit weight of water (Pa m$^{-3}$); and $z$ is the elevation with positive upwards (m). $\theta_l$ and $k_{rw}$ are determined as follows (Van Genuchten, 1980):

$$
\theta_l = \theta_s + S_r (\theta_s - \theta_l)
$$

$$
k_{rw} = \sqrt{S_r \left[1 - \left(1 - S_r^{um}\right)^n\right]^m}
$$

$$
S_r = \frac{\theta_s - \theta_l}{\theta_s - \theta_r} = \left[1 + (a \psi)^n\right]^{-m}
$$

(3),(4),(5)

where $a$ (Pa$^{-1}$), $n$ (dimensionless) and $m$ (dimensionless) are fitting parameters; $\theta_s$ and $\theta_r$ are saturated and residual volumetric water content (dimensionless), respectively; and $\psi$ is soil suction (Pa) and is defined as follows:

$$
\psi = P_g - P_w
$$

(6)

where $P_g$ is gas pressure (Pa).

Vapor flow is mainly affected by two aspects: (i) the gradient of vapor density (Thomas and Sansom, 1995); and (ii) the advective flow of landfill gas. Using the similar approach as liquid water flow, vapor flow is modeled as follows:

$$
\frac{\partial (\rho_v \theta_v)}{\partial t} = -\nabla (\rho_v v_v) - \nabla (\rho_v v_g) + \Gamma_v
$$

(7)

where $\rho_v$ is vapor density (kg/m$^3$); $\theta_v$ is the volumetric vapor content (dimensionless); $v_v$ is the flow velocity of vapor (m/s); $v_g$ is the flow velocity of landfill gas mixture (m/s). Eq. (7) models that the change in mass of vapor is caused by vapor flow ($-\nabla (\rho_v v_v)$), landfill gas flow ($-\nabla (\rho_v v_g)$) and evaporation rate ($\Gamma_v$).

$\rho_v$ is determined as follows (Saito et al., 2006):

$$
\rho_v = \rho_r H_v
$$

(8)

$$
\rho_{r,v} = 10^{-3} T^{-1} \exp (31.37 - \frac{6014.79}{T} - 7.92 \times 10^5 T)
$$

(9)

$$
H_v = \exp \left( -\psi M_{H,O} g / \gamma R_T \right)
$$

(10)

where $\rho_{r,v}$ is the saturated vapor density (kg/m$^3$); $H_v$ is the relative humidity (dimensionless); $R$ is the universal gas constant (8.314 J mol$^{-1}$ K$^{-1}$); $g$ is the gravitational acceleration (9.8 m s$^{-2}$); and $T$ is temperature (K).

$v_v$ can be determined as follows (Saito et al., 2006):

$$
v_v = -K_{vw} \nabla \psi - K_{vs} \nabla T
$$

(11)

$$
K_{vw} = -\frac{D_v}{\rho_l \rho_r H_v} M_{H,O} g
$$

$$
K_{vs} = -\frac{D_v \eta H_v d \rho_{r,v}}{d T}
$$

(12),(13)

where $K_{vw}$ is the isothermal vapor conductivity (m/s); $K_{vs}$ is the non-isothermal vapor conductivity (m$^2$ K$^{-1}$ s$^{-1}$); $D_v$ is the diffusion coefficient of vapor in soil (m$^2$ s$^{-1}$); and $\eta$ is the enhanced factor and is determined as follows:

$$
\eta = 9.5 + 3 \frac{\theta_s}{\theta_r} - 8.5 \exp \left[ -\left( \frac{1 + 2.6 \sqrt{f_c}}{\sqrt{f_c}} \right) \theta_s \right]
$$

(14)

where $f_c$ is clay content in soil (dimensionless).

$D_v$ is determined as follows (Saito et al., 2006):

$$
D_v = \tau D_{vo}
$$

(15)

$$
D_{vo} = 2.12 \times 10^{-4} \left( \frac{T}{273.15} \right)^2
$$

(16)

$$
\tau = \frac{q_{v1}^3}{\theta_s^{2.5}}
$$

(17)

where $D_{vo}$ is diffusion coefficient of vapor in air (m$^2$/s); and $\tau$ is tortuosity (dimensionless).

According to Darcy’s law, $v_g$ is determined as follows:

$$
v_g = -k_{rg} \frac{k_l}{u_l} (\nabla P_g)
$$

(18)

where $k_{rg}$ is the relative gas permeability (dimensionless); and $u_g$ is the viscosity of landfill gas mixture (Pa s). Note that effects of gravity on gas transfer is ignored in Eq. (18), as gas has relatively low density (~1 kg/m$^3$). $k_{rg}$ is given as follows (Parker, 1989):

$$
k_{rg} = \sqrt{1 - S_r \left[1 - S_r^{um}\right]^n}
$$

(19)

The viscosity of a gas mixture $u_g$ is determined as
follows (Reid et al., 1987):

\[
\eta_k = \sum_{i=1}^{a} \frac{y_i u_i}{\sum_{j=3}^{a} y_j \theta_j}
\]

(20)

\[
\theta_k = \left[1 + \left(\frac{u_i}{u_j}\right)^{1/2} \left(\frac{M_i}{M_j}\right)^{1/4}\right] \sqrt{8 \left[1 + \frac{M_i}{M_j}\right]}
\]

(21)

where \(u_i\) is the viscosity of gas \(i\) (Pa s); \(y_i\) and \(y_j\) are molar fractions (dimensionless) of gases \(i\) and \(j\), respectively; \(M_i\) and \(M_j\) are the molar masses of gas \(i\) and \(j\) (kg/mol), respectively.

According to Dalton’s law and ideal gas law (Reid et al., 1987), \(P_g\) can be determined as follows:

\[
P_g = P_{wa} + \sum_{k=1}^{4} c_k R T
\]

(22)

where \(P_{wa}\) is the partial pressure of saturated vapor (Pa), which is depicted in the following form:

\[
P_{wa} = \frac{P_v}{M_{H2O}} = \frac{R}{10^4 M_{H2O}} \exp(31.37 - \frac{6014.79}{T} - 7.92 \times 10^{-3} T)
\]

(23)

The governing equation of moisture flow, which considers both liquid water flow and vapor flow, is obtained by summing the governing equation of liquid water flow (Eq. 1) and that of vapor (Eq. 7):

\[
\frac{\partial \phi \rho \theta + \rho \theta}{\partial t} = -\nabla (\rho \theta_v + \rho_v \theta_v) - \nabla (\rho_v \theta_v) + \rho_v \rho_{H2O}R_l
\]

(24)

2.2 Multi-component gas flow in soil

The governing equation for each gas component (O2, CO2, N2 and CH4) derived by Ng et al. (2015) is adopted as follows:

\[
\frac{\partial}{\partial t} \left[ (\phi - \theta) c_g^k + \theta H_g^k \right] = -\nabla \left( v_g c_g^k \right) - \nabla \left( v_g H_g^k \right) - \nabla N_g^k \pm \rho_{H2O} c_g^k
\]

(25)

where \(\phi\) is soil porosity (dimensionless); \(c_g^k\) is molar concentration of gas \(k\) in gaseous phase (mol/m³; \(k\)=1, 2, 3, 4 represent O2, CO2, N2 and CH4, respectively); \(H_g^k\) is the molar concentration of gas \(k\) dissolved in water (mol/m³); \(N_g^k\) is the diffusive flow of gas \(k\) in gaseous phase (mol/m² s); and \(r_g^k\) is the amount of gas \(k\) involved in MAMO (positive: gas generation; negative: gas consumption). Eq. (25) models that the variation rate of the molar amount of gas \(k\) is caused by advective gas flow in gaseous phase (\(-\nabla (v_g c_g^k)\)), advective flow of dissolved gas in liquid water (\(-\nabla (v_g H_g^k)\)), gas diffusion in gaseous phase (\(-\nabla N_g^k\)) and gas reaction involved in MAMO (\(\pm \rho_{H2O} c_g^k\)).

According to Henry’s law, the gas \(k\) dissolution is determined as follows:

\[
H_g^k = H_g^{k*} c_g^k
\]

(26)

where \(H_g^k\) is Henry coefficient (dimensionless) for gas \(k\).

The diffusive flux \(N_g^k\) is determined as follows:

\[
N_g^k = -D_g^k \nabla c_g^k
\]

(27)

where \(D_g^k\) is the diffusion coefficient (m² s⁻¹) of gas \(k\) in soil and is determined as follows:

\[
D_g^k = \frac{1}{\theta} D_g^k
\]

(28)

where \(D_g^k\) is the diffusion coefficient (m² s⁻¹) of gas \(k\) in a free gas mixture and is determined as follows (Reid et al., 1987):

\[
D_g^k = (1-y_i) \sum_{j=3}^{a} \frac{y_j}{D_{ij}}
\]

(29)

where \(D_{ij}\) is the diffusion coefficient (m² s⁻¹) of the binary mixture of gases \(k\) and \(j\), which is determined as follows (Reid et al., 1987):

\[
D_{ij} = \frac{0.00143 (T+273.15)^{1.75}}{P_g \left(M_{ij} \left(S_{ij}^{1/3} + S_j^{1/3}\right)^2 \right)}
\]

(30)

where \(M_{ij}\) is a combination of the molar mass of gas \(k\) and gas \(j\), given as \(M_{ij} = 2 \left( (M_k^{-1})^3 + (M_j^{-1})^3 \right)^{1/3}\); \(S_k\) and \(S_j\) are the sums of the atomic diffusion volumes or diffusion volumes of simple molecules for each of the gas components (dimensionless; \(S_O2 = 16.3\) for O2; \(S_CO2 = 25.14\) for CH4; \(S_CO2 = 26.9\) for CO2 and \(S_N2 = 18.5\) for N2).

2.3 Heat flow in soil

According to energy balance, heat transfer is modeled using the similar approach as that adopted by Ng et al. (2015):

\[
\frac{\partial}{\partial t} \left[ (\phi - \theta) \rho L + \theta \rho_{H2O} L \right] = -\nabla \left( \rho \nabla T \right) - \nabla Q_{conv} - \nabla Q_{conve} + Q_{sol}
\]

(31)

where \(E\) is the heat capacity of soil (J m⁻³ K⁻¹); \(T_r\) is reference temperature (K); \(L\) is the latent heat of vaporization of water (J/kg); \(\lambda_r\) is thermal conductivity of soil (J m⁻¹ s⁻¹ K⁻¹); \(Q_{conve}\) is sensible heat convection (J m⁻² s⁻¹); \(Q_{conv}\) is latent heat convection (J m⁻² s⁻¹); and \(Q_{sol}\) is heat generation by MAMO (J/m³ s). The thermal conductivity \(\lambda_T\) is determined as follows (Garg and Achari, 2010):

\[
\lambda_T = \lambda_{dry} + S_n (\lambda_{sat} - \lambda_{dry})
\]

(32)

where \(\lambda_{dry}\) and \(\lambda_{sat}\) are the thermal conductivities (J/m s K) of dry soil and saturated soil, respectively. The heat capacity of soil \(E\) is defined as follows (Thomas and Ferguson, 1999):

\[
E = \theta \rho H_1 + (\phi - \theta) \left( \rho_{H2O} + \sum_{k=1}^{a} M_g^k c_g^k H_g^k \right) + (1-\phi) \rho_f H_f
\]
where \( H_l, H_{gv}, H_{gk} \) and \( H_s \) are specific heat capacities (\( J \ kg^{-1} K^{-1} \)) of water, vapor, gas \( k \) and soil particle, respectively; \( M_k^o \) is the molar mass of gas \( k \) (kg/mol); and \( \rho_s \) is soil particle density (kg/m\(^3\)).

The sensible heat convection \( Q_{\text{conv}} \) and latent heat convection \( Q_b \) are determined as follows (Thomas and Ferguson, 1999):

\[
Q_{\text{conv}} = \left( \rho_l H_{vl} + \rho_v H_{gv} + \rho_h H_{ph} + \nu \sum_{i=1}^{4} M_k^o c_i^o H_{gk} \right) (T - T_i)
\]

\[
Q_b = (\rho_v y_v + \rho_h y_h) L
\]

### 2.4 Theoretical formulations for microbial aerobic methane oxidation

According to Ng et al. (2015), the biochemical reaction involved in methane oxidation can be described as follows:

\[
\text{CH}_4 + \text{1.5O}_2 \rightarrow \text{0.5CO}_2 + \text{1.5H}_2\text{O} + 0.5\text{CH}_2\text{O} + \text{Heat}
\]

The methane oxidation rate is mainly affected by water content and temperature in soil. The formulation proposed by Abichou et al. (2011) is adopted to depict methane oxidation rate:

\[
f_{\text{CH}_4}^{\text{CH}_4} = -f_{V,T} f_{V,\text{CH}_4} \frac{V_{\text{max}} y_{\text{CH}_4}}{K_m + y_{\text{CH}_4}} \frac{y_{\text{O}_2}}{K_{\text{O}_2} + y_{\text{O}_2}}
\]

where \( f_{V,T} \) and \( f_{V,\text{CH}_4} \) determine effects of temperature and water content on methane oxidation rate (dimensionless), respectively; \( V_{\text{max}} \) is the maximum methane oxidation rate per unit mass of dry soil (mol/(kg dry soil s)); \( y_{\text{O}_2} \) and \( y_{\text{CH}_4} \) are molar fraction of \( \text{O}_2 \) and \( \text{CH}_4 \), respectively (dimensionless); \( K_m \) and \( K_{\text{O}_2} \) are half saturation constants for \( \text{CH}_4 \) and \( \text{O}_2 \), respectively (dimensionless).

According to Eq. (36), the amount of water and gas reaction by MAMO are determined as follows:

\[
R_i = -1.5 f_{\text{CH}_4}^{\text{CH}_4}
\]

\[
f_{\text{CH}_4}^{\text{CO}_2} = -0.5 f_{\text{CH}_4}^{\text{CH}_4}
\]

\[
f_{\text{CH}_4}^{\text{H}_2\text{O}} = 1.5 f_{\text{CH}_4}^{\text{CH}_4}
\]

Heat generation rate \( Q_{\text{oxi}} \) is given as follows:

\[
Q_{\text{oxi}} = \kappa \rho \omega f_{\text{CH}_4}^{\text{CH}_4}
\]

where \( \kappa \) is the amount of heat generated per mole of methane oxidation (kJ/mol). \( \kappa \) is 632 kJ/mol according to Garg and Achari (2010). Together with Eqs. (1)-(41) forms the theoretical model describing the multi-physical processes involved in methane transfer through landfill cover. The model was solved by finite-element software COMSOL (COMSOL 5.2, 2015).

### 3 VERIFIED BY SOIL COLUMN TEST SIMULATING METHANE OXIDATION

#### 3.1 Soil column test simulating MAMO

The soil column test conducted by Yang (2014) to simulate MAMO in landfill cover was adopted for model verification. The schematic of the experimental setup is shown in Fig. 1. An acrylic cylinder consisting of six sections was used. The top section was flushed with air continuously, while CH4 and CO2 were pumped into the bottom section at the same influx rate of 1.78x10\(^{-4}\) mol/(m\(^2\) s). In between the top and bottom sections, four sections with 0.2-m height each were used to facilitate soil compaction of height 0.8 m. The top 0.3 m of the soil compaction comprised of loess and compost mixture (3% by weight) with a dry density of 1.30 g/cm\(^3\) and a gravimetric water content of 0.20 (volumetric water content of 0.26). The rest 0.5 m of the soil sample was compacted with loess with a dry density of 1.45 g/cm\(^3\) and a gravimetric water content of 0.14 (volumetric water content of 0.20). The measurements include gas concentration, gas pressure and gas emission rate through the column. The test was conducted at room temperature of 20 °C for 40 days. More details of the soil column test can be found in Yang (2014).

#### 3.2 Numerical model setup

As shown in Fig. 2, an axisymmetric numerical model was established based on the configuration of the soil compaction. AD is the axisymmetric line. At AB boundary, zero-flux boundary was set for water transfer, while constant gas concentration for each gas component was specified according to its concentration in the atmosphere (\( c_{\text{CH}_4}^{\infty} = 0.11 \text{mol} / \text{m}^3 \), \( c_{\text{CO}_2}^{\infty} = 9.33 \text{mol} / \text{m}^3 \), \( c_{\text{H}_2\text{O}}^{\infty} = 0 \), \( c_{\text{O}_2}^{\infty} = 31.72 \text{mol} / \text{m}^3 \)). Zero-flux boundary was set at BC boundary for both water and gas transfer. Regarding CD boundary, zero-flux boundary was set for water transfer, \( \text{O}_2 \) and \( \text{N}_2 \) transfer, while a constant influx
of $1.78 \times 10^{-4}$ mol/(m$^2$ s) was specified for both CH$_4$ and CO$_2$ transfer. For heat transfer, constant temperature of 20 °C was set at AB, BC, and CD boundaries. The initial volumetric water content of 0.26 and 0.20 were specified at ABFE area and EFCD area. The initial gas concentration for each gas component was set according to its concentration in the atmosphere, while the initial temperature was 20 °C. Transient numerical simulation was conducted for 40 days. Table 1 shows the input parameters, which were either measured by Yang (2014) or estimated from literature.

## Table 1. Input parameters for numerical simulation.

| Zone     | Parameter                              | Value          |
|----------|----------------------------------------|----------------|
| ABFE     | Dry density (kg/m$^3$)                  | 1.30           |
|          | Intrinsic permeability ($10^{-12}$ m$^2$) | 1.20           |
|          | Van Genuchen fitting parameters $a$ ($10^{-8}$ Pa$^{-1}$) | 0.072          |
|          | Van Genuchen fitting parameters $m$     | 1.132          |
|          | Van Genuchen fitting parameters $n$     | 0.614          |
|          | Thermal conductivity of dry soil (J/(s m K)) | 0.40           |
|          | Thermal conductivity of wet soil (J/(s m K)) | 2.03          |
|          | The maximum methane oxidation rate (mol/(kg s)) | $3.35 \times 10^{-7}$ |
|          | Dry density (kg/m$^3$)                  | 1.450          |
|          | Intrinsic permeability ($10^{-15}$ m$^2$) | 2.20           |
|          | Van Genuchen fitting parameters $a$ ($10^{-8}$ Pa$^{-1}$) | 0.032          |
|          | Van Genuchen fitting parameters $m$     | 1.05           |
|          | Van Genuchen fitting parameters $n$     | 0.72           |
|          | Thermal conductivity of dry soil (J/(s m K)) | 0.44           |
|          | Thermal conductivity of wet soil (J/(s m K)) | 2.03          |
|          | The maximum methane oxidation rate (mol/(kg s)) | $6.00 \times 10^{-8}$ |

4.2 Establishment of numerical model

An axisymmetric numerical model (Fig. 6) was built based on the configuration of the soil column. AD is the axisymmetric line. Regarding for moisture transfer, evaporation rate was specified at AB boundary for moisture transfer, while zero-flux boundary was set at BC and CD boundary. For gas transfer, constant gas
concentration was set at AB boundary for each gas component according to its concentration in the atmosphere (i.e., the molar concentration of CH$_4$, CO$_2$, O$_2$ and N$_2$ are 0, 0.011, 9.33, 31.72 mol/m$^3$, respectively), while zero-flux was applied at BC and CD boundaries. As for heat transfer, heat flux was specified at AB and BC boundaries, while a constant temperature of 70 °C as applied in the test was set at CD boundary.

The heat fluxes specified at AB and BC boundaries are determined as follows (Liu, 2006):

$$Q_h = h(T - T_a)$$  \hspace{1cm} (42)

where $Q_h$ is heat flux ($W/m^2$); $T$ and $T_a$ are soil temperature and atmospheric temperature ($K$), respectively; and $h$ is heat exchange coefficient between solid surface and air ($W/m^2K$). When wind is negligible, $h$ equals 6.06 $W/(m^2K)$ in the present study.

The evaporation rate $\Gamma_{ev}$ set at AB boundary is determined as follows (Wilson et al., 1997):

$$\Gamma_{ev} = (0.027 + 0.0156V_{wind} + 0.0025(T - T_a)) \times \left( \frac{P_{vsa} - P_{H_2O}}{P_{vsa} - P_{H_2O}} \right) \times 100$$  \hspace{1cm} (43)

where $P_{vsa}$ is the vapor pressure in the atmosphere (Pa); and $V_{wind}$ is the wind velocity (m/s), which is ignored in this study.

The input soil properties are the same as those in the bottom soil layer in Yang’s soil column test (i.e., EFCD in Table 1), except the maximum methane oxidation rate was set as zero due to negligible methane oxidation capacity. The physical properties of water and gas are the same with those in ABCD in Table 1.

### 4.3 Verification results

Fig. 7 shows the temporal variation of soil temperature at different elevations of column. The measured and computed results are consistent. After heating for 1 day, the soil temperature at each elevation increased quickly and kept almost constant afterwards. As elevation increases from 0.1 m to 0.3 m, noticeable reduction in soil temperature could be observed. As elevation further increased, the soil temperatures at each elevation were quite closed. This is due to the heat dissipation through the side-wall of soil column.

Fig. 8 shows that the temporal variation of soil suction at different elevations of column are consistent. Interestingly, both measured and computed soil suction at elevation of 0.7 m decreased after heating for 1 day. This is likely due to the vapor condensation. Afterwards,
the soil suction increased as heating continued. Overall, the measured and computed results are consistent. The largest difference occurred at the elevation of 0.7 m, where the measurements are larger than the computed. This indicates the underestimation of evaporation rate by Eq. (43). A possible reason could be due to the fluctuation of relative humidity during test.

5 CONCLUSIONS

A new theoretical model was developed to consider effects of vapor flow and temperature gradient on soil hydrological response and gas distributions during coupled water-gas-heat reactive transfer in unsaturated soil. The model was implemented in a finite element software COMSOL. Thereafter, the model was verified by (i) a published soil column test simulating methane oxidation; and (ii) a soil column test subject to heating. Reasonable agreement between the measured and computed results could be obtained, including multi-component gas concentration, suction, gas pressure, and soil temperature etc. The model provides a tool for investigating methane transfer through landfill covers.

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