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Modelling non-isothermal volume change and solute transport behaviours of a semi-permeable clay soil under the combined influence of mechanical loading, chemical-osmosis, and thermo-osmosis

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Abstract: Clays are widely used in geotechnical and geoenvironmental engineering applications and it is crucial to understand its behaviour for the dynamic field conditions. The presence of a temperature gradient across clayey soils that exhibit semi-permeable membrane (or osmotic) behaviour may promote a number of complex processes, including thermal expansion or consolidation, thermally induced osmosis, thermal diffusion, along with other flow and deformation processes. Chemical-osmosis and chemico-osmotic consolidation that are significant in isothermal conditions are also affected by temperature. Publications on chemical-osmosis, and to some extent thermo-osmosis behaviour of semi-permeable clays under coupled conditions are widely available. However, studies that include the influence of both thermo-osmosis and chemical-osmosis together are rare. In this paper, a fully coupled numerical model is presented to study the effects of both osmotic processes on thermo-hydro-mechanical-chemical behaviour of semi-permeable clays. Solute spread in a landfill clay liner is investigated under the
combined influence of mechanical, thermal, and chemical loading. Model results show that the clay
deformation is sensitive to thermo-osmosis; and the effects of thermo-osmotic consolidation, excess pore
water dissipation, and the overall settlement increases with temperature. Variation of the source
temperature from 40°C to 80°C yielded an increase of 11.3% of the peak soil settlement. Significant
contribution of thermo-osmosis on solute transport is noticed in this study and ignoring the process
substantially deviate from the realism. Up to 80% overprediction of cadmium spread is observed in the
clay liner when the thermo-osmotic processes are neglected.

**Keywords:** coupled transport, deformation, temperature, osmotic conductivity, thermo-osmotic
conductivity, sorption.

1 Introduction

Clayey soils are often used as buffer materials to prevent and to minimise the spread of toxic
pollutants in the surrounding environment. Materials such as synthetic or natural clay liners, compacted
clays, often constitute the key component of engineered barrier systems (Coo et al., 2016) in various
waste disposal and landfill applications. Efficacy of such systems depends largely on ensuring the
expected physical, chemical and mechanical behaviour of clay buffers in-field or in-situ conditions
(Zheng et al, 2017), where they are exposed to simultaneous thermal, hydraulic, chemical and mechanical
loading events. Therefore, it is essential to study their complex, coupled flow and deformation behaviours
on mitigating contaminant spread effectively and/ maintaining contamination level below regulatory
limits.

Coupled flow and deformation processes in clays that exhibit semi-permeable membrane behaviour
are complex and strongly affected by the osmotic processes related to the physico-chemical interactions between the clay aggregates and the pore fluid (Barbour and Fredlund, 1989). During osmosis fluid flows through a semi-permeable membrane submitted to pore fluid chemicals (solutes) concentration gradients (Mitchell, 1973; Keijzer, 1997; Malusis, 2003) or to soil thermal gradient (Mitchell and Soga, 2005); and may lead to volumetric changes in the soil. The former is known as chemical-osmosis and the later as thermo-osmosis. The corresponding soil deformations are termed as chemico-osmotic consolidation (Mitchell, 1973; Kaczmarek and Hueckel, 1998) and thermo-osmotic consolidation (Mitchell and Soga, 2005). Osmotic potentials in clays depend on the osmotic efficiency of the membrane \( \omega \), which varies between \( 0 \leq \omega \leq 1 \) (Shackelford et al., 2019). Unlike perfect semi-permeable membranes, \( \omega = 1 \), clays exhibit imperfect semi-permeable behaviour and that leads to solute as well as pore fluids flow across the membrane (Barbour and Fredlund, 1989). When exposed to heating both soil aggregates and pore fluid experience thermal dilation; and under drained condition, the thermally induced expansion and expulsion of pore fluid across the membrane result into consolidation of the soil volume (Paaswell, 1967; Habibagahi, 1977; Delage, 2000; Monfared et al., 2012; Donna and Laloui, 2015). Pore fluid flow in semi-permeable clays during chemical-osmosis and thermo-osmosis are measured by the osmotic conductivity \( k_\omega \) and the thermo-osmotic conductivity \( k_T \), respectively (Goncalves et al., 2012; Shackelford et al., 2019). When submitted to simultaneous thermal, hydraulic and chemical gradients, they combinedly contribute with the hydraulic conductivity \( k_h \) into the bulk fluid flow. Accurate prediction/estimation of transport and fate of solutes in semi-permeable clays, therefore, depends on comprehensive understanding of the combined, inter-related flow and deformation behaviours.

Numerous studies on coupled processes in clayey soils are available in the literature. Here the focus is on the theoretical and/numerical studies including coupled thermal, hydraulic, mechanical and/
chemical processes in semi-permeable clays with particular relevance to osmotically induced volume change behaviours. For isothermal conditions, the effects of chemical-osmosis and chemico-osmotic consolidations on coupled flow processes are presented in the works of Mitchell et al. (1973), Barbour and Fredlund (1989), Kaczmarek and Hueckel (1998), Malusis and Shackelford (2002), Peters and Smith (2004), Lewis et al. (2009), Pu et al. (2016), Xie et al. (2015), Zhang et al. (2018) and others (a comprehensive list of the literatures are available in Zhang et al. (2018)). However, the contribution of thermo-osmosis on coupled flow processes is usually ignored based on the assumption that the thermo-osmotic flux is negligible (Sánchez, et al., 2016; Shackelford et al., 2019). For argillaceous media e.g. semi-impermeable clays, validity of this assumption is questionable (Soler, 2001; Shackelford et al., 2019). Laboratory investigations on non-isothermal volume change experiments in clays, (Carnahan, 1983; McVay, 1984, Delage et al., 2000; Trémosa et al., 2010; Goncalves et al., 2012; Roshan et al., 2015), reported significant mass transfer associated with thermo-osmosis. Nevertheless, literatures including thermo-osmosis in coupled flow processes are limited (Zhai et al., 2020). Relevant analytical and/numerical modelling studies include, McTigue (1986), Smith and Booker (1993), Zhou et al. (1998), Ekbote and Abousleiman (2005), Villar et al. (2005), Tong et al. (2010), Gonçalvês and Trêmosa (2010), Goncalves et al. (2012), Yang et al. (2014), Roshan et al. (2015), Gao et al. (2017), Zheng et al. (2015), Salomoni (2018), Song et al. (2019), Sun et al. (2020), Zhai et al. (2020). These studies investigated the contribution of temperature driven osmotic processes on partially- or fully-coupled thermo-hydraulic-mechanical (THM) or thermo-hydraulic-chemical-mechanical (THCM) behaviours, but ignored chemical-osmosis or chemico-osmotic consolidation. Ekbote and Abousleiman (2005) developed a coupled thermo-hydraulic-chemical-mechanical model to study the thermochemical effects on borehole stability in oil and gas exploration applications. Poulet et al. (2012) also derived a coupled THCM model
to investigate the influence of folds, shear zones, and other geological structures on hydrothermal ore-
deposits formation. To study the impacts of temperature on the alteration of chemical properties such as
illitization of engineered barriers, Zheng et al. (2015) presented a coupled THCM model including stress
balance, enthalpy balance, fluid and solute mass conservation principles. However, Ekbote and
Abousleiman (2005) and Poulet et al. (2012) did not consider the influence of thermo-osmosis on solute
transport. Although Zheng et al. (2015) considered the thermo-osmotic effects on solute transport, they
ignored the contribution of thermal diffusion on solute transport and chemico-osmotic consolidations on
the overall soil deformation. None of these models can directly calculate the soil deformation or
settlement due to partial coupling or neglecting. Literatures that include both chemical-osmosis and
thermo-osmosis behaviours in fully coupled THCM problems are rarely available.

In this work, the effects of both thermal and chemical osmosis on deformation and solute transport
behaviours of a saturated, natural, semi-permeable clay liner are investigated. Previously presented model
of Zhang et al. (2018), to study coupled hydro-mechanical-chemical behaviours of saturated natural clays
including chemical-osmosis and chemico-osmotic consolidation, is extended here by including the non-
isothermal flow and deformation behaviours. Unlike the previous models (Ekbote and Abousleiman, 2005;
Poulet et al., 2012; Zheng et al., 2015), the presented model can directly calculate the soil settlement
behaviour of semipermeable clays subjected to multiple loading mechanisms. It also includes thermal
diffusion or Soret effect, and both chemico-osmotic and thermo-osmotic consolidation effects under a
fully coupled modelling framework. Therefore, the presented model addresses the limitations of the
previous models, and advances the knowledge and understanding of non-isothermal behaviours of
semipermeable clay soils. In this paper, three loading mechanisms, namely, i) Mechanical loading,
associated with a landfill-waste weight; ii) chemical loading, due to osmotic potential; and iii) thermal
loading, as a result of thermal gradient, are incorporated with simultaneous fluid, heat and solute transport mechanisms. Both molecular diffusion and thermal diffusion, and sorption processes on the solute transport behaviours are considered. The thermo-chemo-poroelastic model considers a homogenous, isotropic porous media with linear and elastic deformation. The accuracy of the model to predict non-isothermal volume change behaviours is demonstrated by validating the model against laboratory experiments obtained from the literatures. Applications of the model include a comparative analysis of the osmotic processes on soil deformation behaviour, and non-isothermal evolution of pore fluid pressure, overall settlement as well as transport and fate of a solute in a semi-permeable clay soil. The aim of this study is to present a quantitative analysis of the thermo-osmotic processes related to non-isothermal, coupled flow and deformation problems, and to investigate its relative importance on regulating volume change and solute transport behaviours when multiple loading events occur simultaneously.

2 Theoretical background

The governing equations of flow and deformation, presented here, are for one-dimensional (1D) problems. The following assumptions are made: (1) soil is homogeneous, isotropic and saturated; (2) movements occur only in the vertical direction; (3) transport of pore fluid and solutes can be explained via Darcy’s law and Fick’s law, respectively; and (4) the consolidation deformation of soil is linear and elastic.

2.1 Governing equations of soil deformation

The equilibrium between total stress ($\sigma_z$) and body force ($f$) in a small deforming soil sample is written as,

$$\frac{\partial \sigma_z}{\partial z} + f = 0$$  (1)
\[ f = [n\rho_f + (1 - n)\rho_s]g \quad (2) \]

Where the subscript \( z \) denotes the vertical direction, \( n \) is porosity, \( g \) is the gravitational acceleration, \( \rho_f \) and \( \rho_s \) are the densities of pore fluid and soil solids, respectively. The principle of effective stress \((\sigma'_z)\) dictates that

\[ \sigma'_z = \sigma_z - u \quad (3) \]

where \( u \) is the pore fluid pressure. Influences of three loading mechanisms, e.g., mechanical, chemical and thermal loading, on the soil deformation is considered. Following (Zhang et al., 2018), the constitutive relationship of soil can be further described as,

\[ \sigma'_z = \frac{E(1 - v)}{(1 - 2v)(1 + v)}(\varepsilon_z - \varepsilon_\pi - \varepsilon_T) \quad (4) \]

where \( E \) is the Young’s modulus of elasticity, \( v \) is Poisson’s ratio, \( \varepsilon_z \) is the total strain. \( \varepsilon_\pi \) and \( \varepsilon_T \) represent the strains associated with chemico-osmotic consolidation and thermo-osmotic consolidation, respectively. The total strain \((\varepsilon_z)\) is expressed in terms of soil vertical displacement \((w_z)\) as,

\[ \varepsilon_z = -\frac{\partial w_z}{\partial z} \quad (5) \]

The osmotic strain is related to the osmotic potential, i.e., the osmotic suction \((\pi)\), and in an incremental form it is expressed as (Barbour and Fredlund, 1989),

\[ d\varepsilon_\pi = -m_\pi d\pi \quad (6) \]

where \( m_\pi \) is the coefficient of volume change due to the osmotic pressure gradient, and \( \pi = RTc \). Here, \( R \) is the universal gas constant, \( T \) is absolute temperature in degree Kelvin and \( c \) is the solute concentration in the liquid phase. For non-isothermal condition, Eq. (6) is expanded as,

\[ d\varepsilon_\pi = -m_\pi d(RTc) = -m_\pi Rdc - m_\pi Rc dT. \quad (7) \]

For a thermo-elastic porous medium, the thermally induced strain is expressed after Robinet et al. (1996) as,
\[ \varepsilon_T = -\alpha dT - \beta_f^T dT \]  

(8)

where \( \alpha \) is the thermal expansion coefficient of the soil aggregates and \( \beta_f^T \) is the thermal expansion coefficient of the pore fluid.

Substitution of Eqs. (2)-(8) into Eq. (1) yields,

\[
\frac{E(1-\nu)}{(1+\nu)(1-2\nu)} \left[ -\frac{\partial^2 w_z}{\partial z^2} + m_s RT \frac{\partial c}{\partial z} + (m_s R c + \alpha + \beta_f^T) \frac{\partial T}{\partial z} \right] + \frac{\partial u}{\partial z} + [(1-n)\rho_s + n \rho_f]g = 0
\]

(9)

Eq. (9) is the governing equation of soil deformation, which includes four independent variables, e.g., soil displacement \( w_z \), excess pore fluid pressure \( u \), chemical concentration \( c \) and temperature \( T \).

2.2 Governing equations of pore fluid flow

The mass conservation equation of pore fluid flow is written as (Smith, 2000),

\[
\frac{\partial (\rho_f n)}{\partial t} + \nabla (\rho_f n V_f) = 0
\]

(10)

where \( V_f \) is the absolute velocity of the pore fluid. The Eq. (10) is expanded as,

\[
\rho_f \frac{\partial n}{\partial t} + n \frac{\partial \rho_f}{\partial t} + \nabla (\rho_f n V_f) = 0.
\]

(11)

Francois (2009) suggested that the temporal variation of pore fluid density can be expressed as a function of pore fluid pressure \( u \) and temperature \( T \). By assuming that the influence of solute concentration on pore fluid density is negligible, the temporal variation can be described as,

\[
\frac{\partial \rho_f}{\partial t} = \rho_f \beta_f \frac{\partial u}{\partial t} - \rho_f \beta_f^T \frac{\partial T}{\partial t}
\]

(12)

where \( \beta_f \) is the compressibility of the pore fluid.

In this study, the change in soil volume is being coupled with three loading mechanisms, e.g. mechanical, chemical and thermal loadings. For isothermal conditions, Kaczmarek and Hueckel (1998) proposed a relationship for porosity variation of semi-permeable clays, by incorporating mechanical
loading and chemical loading. Here, the relationship is extended by including the thermal and thermo-
osmotic consolidations as,

\[ n = n_0 - \Delta n = n_0 - m_v \Delta \sigma_z' - m_e RT \Delta c - m_e Rc \Delta T - \alpha \Delta T - \beta_T \Delta T \]  

(13)

where \( m_v \) is the volume change coefficient related to the effective stress. The temporal derivative of Eq. (13) is expressed as,

\[ \frac{\partial n}{\partial t} = m_v \frac{\partial u}{\partial t} - m_e RT \frac{\partial c}{\partial t} - \left( m_e Rc + \alpha + \beta_T \right) \frac{\partial T}{\partial t} \]  

(14)

The absolute pore fluid velocity (\( V_f \)) combines the pore fluid relative velocity with respect to the soil skeleton (\( V_r \)) and the absolute velocity of the soil-skeleton deformation (\( V_s \)) as,

\[ V_f = V_r + V_s \]  

(15)

\[ V_r = \frac{1}{n} V \]  

(15a)

\[ V_s = \frac{\partial w_z}{\partial t} \]  

(15b)

where \( V \) is the velocity of the pore fluid flow and it combines the contributions of hydraulic head, osmotic-pressure head and temperature gradients. Gonçalvês and Trémosa (2010) explained the thermo-osmotically driven pore fluid flow as,

\[ V_T = \frac{k_T}{\mu_i(T)} \frac{\partial T}{\partial z} \]  

(16)

where \( V_T \) is the pore fluid velocity associated with the temperature gradient and \( k_T \) is the thermo-osmotic conductivity. \( \mu_i(T) \) is the temperature-dependent dynamic viscosity of water.

Fluid flow due to hydraulic head gradient (\( V_u \)) and osmotic-pressure head gradient (\( V_n \)) are presented in Smith (2000) and Zhang et al. (2018). Here, the relationship is extended by including \( V_T \) as,

\[ V = V_u + V_n + V_T = -\frac{k_h \partial u}{\gamma_w \partial z} + \omega \frac{RT k_h \partial c}{M \gamma_w \partial z} + \frac{k_T}{\mu_i} \frac{\partial T}{\partial z} \]  

(17)

where \( k_h \) is in-situ hydraulic conductivity, \( \gamma_w \) is the unit weight of water, \( M \) is the molar mass, and \( \omega \) is the osmotic efficiency. Here, \[ \omega \frac{RT k_h}{M \gamma_w} = k_\omega \], i.e., the osmotic conductivity. Hart and John (1986)
described the in-situ hydraulic conductivity \( (k_h) \) in terms of initial hydraulic conductivity \( (k_{h0}) \) and initial porosity \( (n_0) \) as,

\[
k_h = k_{h0} \left( \frac{n}{n_0} \right)^3
\]  

(18)

Substituting Eqs. (12), (14) and (17) into Eq. (11) yields the governing equation of pore fluid flow,

\[
(m_v + n\beta_f) \frac{\partial u}{\partial t} - m_nRT \frac{\partial c}{\partial t} - (m_nRC + \alpha + n\beta_f) \frac{\partial T}{\partial t} = -\frac{\partial}{\partial z} \left[ -k_h \frac{\partial u}{\partial w} + \frac{RT}{\gamma_w} \frac{\partial c}{\partial z} + \frac{k_\tau}{\mu_l} \frac{\partial T}{\partial z} - n \frac{\partial w}{\partial z} \right]
\]  

(19)

2.3 Governing equations of heat transfer

Following the energy conservation law heat transport in soil, in absence of a source/sink, is written as,

\[
\frac{\partial \Phi}{\partial t} = -\frac{\partial Q}{\partial z}
\]  

(20)

where \( Q \) is the heat flux per unit volume of soil and \( \Phi \) is the heat content. Considering that the different components of the soil are in thermal equilibrium, heat content is expressed as (Thomas and Cleall, 1999),

\[
\Phi = [(1 - n)C_{ps}\rho_s + nC_{pf}\rho_f](T - T_r)
\]  

(21)

where \( C_{ps} \) and \( C_{pf} \) are the specific heat capacity of the solid particles and pore liquid, respectively, and \( T_r \) is the reference temperature.

We consider two modes of heat transfer in soil, e.g., thermal conduction and convection. The heat flux is therefore expressed as,

\[
Q = -\lambda_T \frac{\partial T}{\partial z} + C_{pf}\rho_f V(T - T_r)
\]  

(22)

where \( \lambda_T \) is the intrinsic thermal conductivity of the soil.

Substitution of Eqs. (21)-(22) into Eq. (20) yields the governing heat transfer equation as

\[
A \frac{\partial T}{\partial t} + B \frac{\partial u}{\partial t} + C \frac{\partial c}{\partial t} = -\frac{\partial}{\partial z} \left[ -k_h \frac{\partial u}{\gamma_w} + \frac{RT}{\gamma_w} \frac{\partial c}{\partial z} + \frac{k_\tau}{\mu_l} \frac{\partial T}{\partial z} \right]
\]  

(23)
\[ A = C_{ps} \rho_s + [n - (T - T_r)(m_\pi Rc + \alpha)][(C_{pf} \rho_f - C_{ps} \rho_s) - (T - T_r)nC_{pf} \beta_f^T] \tag{23a} \]

\[ B = (T - T_r)(C_{pf} \rho_f m_v - C_{ps} \rho_s m_v + nC_{pf} \beta_f) \tag{23b} \]

\[ C = (T - T_r)(C_{pf} \rho_f - C_{ps} \rho_s)m_R T \tag{23c} \]

2.4 Governing equations of solute transport

Transport of a solute in pore fluid is explained as,

\[ \frac{\partial (nc)}{\partial t} = -\frac{J_f}{\partial z} + Y \tag{24} \]

where \( J_f \) is the total solute flux in the pore fluid, and \( Y \) is the sink/source term. The total flux combines convection, molecular diffusion and thermal diffusion and it is expressed as,

\[ J_f = J_c + J_{D_c} + J_{D_T} \tag{25} \]

where \( J_c \), \( J_{D_c} \), and \( J_{D_T} \) represent solute flux due to convection, molecular diffusion and thermal diffusion, respectively. They are defined as,

\[ J_c = cV = c \left( (1 - \omega) \left( -\frac{k_h \partial u}{\gamma_w \partial z} \right) + \omega \frac{k_h RT \partial c}{\gamma_w MT \partial z} + \frac{k_T \partial T}{\mu_l \partial z} \right) \tag{26} \]

\[ J_{D_c} = -nD_c \frac{\partial c}{\partial z} \tag{27} \]

\[ J_{D_T} = -n\tau D_0 S_T c \frac{\partial T}{\partial z} \tag{28} \]

where \( D_c \) is the effective diffusion coefficient, \( D_0 \) is the diffusion coefficient of the solute in free liquid.

Eq. (28) calculates the contribution of temperature on the solute diffusion, i.e., the Soret effect, and \( S_T \) is the Soret coefficient. \( \tau \) is the tortuosity factor and it lies between \( 0 < \tau < 1 \). In this work, \( \tau \) is calculated following Liu et al. (2004) as,

\[ \tau = n^2 \tag{29} \]

Malusis et al. (2015) described the effective diffusion coefficient of semipermeable clays as,
\[ D_c = \tau (1 - \omega) D_0 \quad (30) \]

Substitution of Eqs. (25)-(30) into Eq. (24) yields
\[
\frac{\partial (n\epsilon)}{\partial t} = -\frac{\partial}{\partial z}\left(1 - \omega \right)\left(-\frac{k_h}{\gamma_w} \frac{\partial u}{\partial z} \right) c + \omega \frac{RT}{M} \frac{k_h}{\gamma_w} \frac{\partial c}{\partial z} c + \frac{k_T}{\mu_i} \frac{\partial T}{\partial z} c - nD_c \frac{\partial c}{\partial z} c - n\tau D_0 S_T c \frac{\partial T}{\partial z} \pm Y \quad (31) \]

Eq. (31) is the governing equation of solute transport in the pore fluid.

The mass conservation equation of a solute adsorbed in soil aggregates is written as,
\[
\frac{\partial [(1-n)\rho_s S]}{\partial t} = -\frac{\partial J_s}{\partial z} \pm Y \quad (32) \]

where \( S \) represents the amount of solute adsorbed in the solid phase. \( J_s \) is the solute flux in the solid phase, which is expressed as,
\[ J_s = (1 - n)V_s \rho_s S. \quad (33) \]

Here, solid-solution partitioning is described as,
\[ S = K_d c \quad (34) \]

where \( K_d \) is the partitioning or distribution coefficient.

Substitution of Eqs. (33)-(34) into Eq. (32) yields
\[
\frac{\partial [(1-n)\rho_s K_d c]}{\partial t} = -\frac{\partial}{\partial z}\left[ (1 - n) \frac{\partial u_s}{\partial t} \rho_s K_d c \right] \pm Y \quad (35) \]

which is the governing equation of solute transport in the solid phase.

According to the mass balance of solute, combining Eq. (31) and (35) together, then
\[
\frac{\partial (n\epsilon)}{\partial t} + \frac{\partial [(1-n)\rho_s K_d c]}{\partial t} = -\frac{\partial}{\partial z}\left(1 - \omega \right)\left(-\frac{k_h}{\gamma_w} \frac{\partial u}{\partial z} \right) c + \omega \frac{RT}{M} \frac{k_h}{\gamma_w} \frac{\partial c}{\partial z} c + \frac{k_T}{\mu_i} \frac{\partial T}{\partial z} c - nD_c \frac{\partial c}{\partial z} c - n\tau D_0 S_T c \frac{\partial T}{\partial z} - n\tau D_0 S_T \frac{\partial T}{\partial z} c + \frac{\partial J_s}{\partial z} \pm Y + \frac{n\tau D_0 S_T c}{\partial z} \frac{\partial T}{\partial z} c \quad (36) \]

Eq. (36) is the final governing equation of solute transport in a porous medium.

**3. Model validation**
Partial validation of the model is presented in this section. Full model validation could not be performed due to lack of experimental data. The accuracy of the model on predicting thermo-osmosis and the influence of thermal gradient on solute transport has been tested here by comparing with relevant experimental data obtained from the literature. More validation and verification of the model, especially the chemical-osmosis processes are presented in Zhang et al. (2018). The model simulations have been carried out using the COMSOL Multiphysics (https://www.comsol.com) software.

3.1 Comparison with the results of Delage et al. (2000)

Delage et al. (2000) conducted experimental investigation on temperature induced volume change of clay-water system and subsequent consolidation in saturated Boom clays. Samples (76 mm height and 38 mm diameter) were tested in a triaxial compression cell under a constant isotropic stress of 4 MPa and temperatures up to 100°C. Thermal dilation and expulsion of porewater from the samples during the drained consolidation tests allowed the thermo-osmotic consolidation to take place. Here the model predicted results have been compared with the thermal volume change behaviour of the clay-water system observed in their experiment. To account thermal dilation, Baldi et al. (1988) expressed the porewater thermal expansion coefficient \( \beta_f(T,u) \) as a function of temperature and water pressure as,

\[
\beta_f(T,u) = \alpha_0 + (\alpha_1 + \beta_1 T) \ln(mu) + (\alpha_2 + \beta_2 T)(\ln(mu))^2
\]

(37)

where \( \alpha_0 (=4.505 \times 10^{-4} \text{ °C}^{-1}) \), \( \alpha_1 (=9.156 \times 10^{-5} \text{ °C}^{-1}) \), \( \alpha_2 (=6.381 \times 10^{-6} \text{ °C}^{-1}) \), \( \beta_1 (= -1.2 \times 10^{-6} \text{ °C}^{-2}) \), \( \beta_2 (= -5.766 \times 10^{-8} \text{ °C}^{-2}) \), \( m (=15 \text{ MPa}^{-1}) \) are constants.

Table 1 Parameters used to compare simulation results against the result of Delage et al. (2000)

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Values</th>
<th>References</th>
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<tbody>
<tr>
<td>( \alpha_0 )</td>
<td>( =4.505 \times 10^{-4} \text{ °C}^{-1} )</td>
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<tr>
<td>( \alpha_1 )</td>
<td>( =9.156 \times 10^{-5} \text{ °C}^{-1} )</td>
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<tr>
<td>( \alpha_2 )</td>
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<td>( m )</td>
<td>( (=15 \text{ MPa}^{-1}) )</td>
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</table>
The parameters used in the validation exercise are listed in Table 1. The initial temperature \( T(z, 0) = 240 \) K, \((0 \leq z < L = 0.076 \text{ m})\), while the boundary temperature \( T(L, t) = 373 \) K \((t \geq 0)\). The porewater pressure remained constant throughout the simulation, i.e. \( u(z, t) = 4 \) MPa, \((0 \leq z \leq L \text{ and } t \geq 0)\). The simulation time \((t)\) is 266.67 h.

The results are presented in Fig.1. The model predicted result shows good agreement with the experimental result. Temperature induced porewater expansion and expulsion caused the sample to contract and, therefore, reduced its porosity. The decreased volume or porosity reduction is associated with the dissipation of porewater pressure. Delage et al. (2000) conducted four tests using the same sample. Here we compared the ‘Test 1’ results which was suggested as better quality than the other test.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial porosity, ( n_0 )</td>
<td>0.370</td>
<td></td>
</tr>
<tr>
<td>Initial hydraulic conductivity, ( k_{h0} )</td>
<td>(2.0 \times 10^{-12} ) ms(^{-1})</td>
<td>Delage et al. (2000)</td>
</tr>
<tr>
<td>Coefficient of volume change, ( m_v )</td>
<td>(1 \times 10^{-5} ) Pa(^{-1})</td>
<td>Delage et al. (2000)</td>
</tr>
<tr>
<td>Unit weight of liquid, ( \gamma_w )</td>
<td>10 kNm(^{-3})</td>
<td></td>
</tr>
<tr>
<td>Density of the soil, ( \rho_s )</td>
<td>2600 kgm(^{-3})</td>
<td></td>
</tr>
<tr>
<td>Modulus of elasticity, ( E )</td>
<td>200 MPa</td>
<td>Francois et al. (2009)</td>
</tr>
<tr>
<td>Poisson’s ratio, ( \nu )</td>
<td>0.3</td>
<td>Peters and Smith (2004)</td>
</tr>
<tr>
<td>Thermal expansion coefficient of soil, ( \alpha )</td>
<td>(1 \times 10^{-5} ) °C(^{-1})</td>
<td>Delage et al. (2000)</td>
</tr>
<tr>
<td>Compressibility of pore liquid, ( \beta_c )</td>
<td>(4.5 \times 10^{-10} ) Pa(^{-1})</td>
<td>Francois et al. (2009)</td>
</tr>
<tr>
<td>Specific heat capacity of soil, ( C_{ps} )</td>
<td>(2.85 \times 10^6 ) Jm(^{-3})K(^{-1})</td>
<td>Delage et al. (2000)</td>
</tr>
<tr>
<td>Specific heat capacity of pore liquid, ( C_{pf} )</td>
<td>4186 Jkg(^{-1})K(^{-1})</td>
<td>Francois et al. (2009)</td>
</tr>
<tr>
<td>Intrinsic thermal conductivity of soil, ( \lambda_T )</td>
<td>1.7 Wm(^{-1})K(^{-1})</td>
<td>Delage et al. (2000)</td>
</tr>
</tbody>
</table>
results (that exhibited anomalies at lower temperature regimes). The deviation observed at higher temperatures (70-100°C), where the model under-estimated the rate of porosity reduction (or porewater pressure dissipation), may be due to the uncertainties associated with the additional model parameters used in the simulation.

![Graph a) showing porosity and thermal volumetric strain](image1)

![Graph b) showing temperature and thermal volumetric strain](image2)
Figure 1 Comparison of model predicted result of temperature induced (a) porosity and drained water variation and (b) thermal volumetric strain with that of the Delage et al. (2000).

3.2 Comparison with the results of Do et al. (2006)

Do et al. (2006) investigated effects of temperature on zinc ($Zn^{2+}$) and cadmium ($Cd^{2+}$) diffusion in natural clays collected from southwester Korea. Laboratory soil column tests were conducted at various temperatures ranging from 15°C to 55°C. Here, the results are compared with the experiments conducted at 55°C. 100 mm by 50 mm solute free clay samples were exposed, individually, to a source concentration of 500 mg L$^{-1}$ $Zn^{2+}$ and 300 mg L$^{-1}$ $Cd^{2+}$ and their transport in the soil columns were observed for 30 days.

<table>
<thead>
<tr>
<th>Table 2</th>
<th>Simulation conditions to test against the results of Do et al. (2006)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial</td>
<td>$c(z,0) = 0$ $T(z,0) = 273$ K $(0 &lt; z &lt; L)$</td>
</tr>
<tr>
<td>Boundary</td>
<td>$c(0,t) = c_0$ $T(0,t) = 328$ K $(t \geq 0)$</td>
</tr>
<tr>
<td>conditions</td>
<td>$rac{\partial c}{\partial x}(L,t) = 0$ $T(L,t) = 273$ K $(t \geq 0)$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 3</th>
<th>Parameters used to compare simulation results against the result of Do et al. (2006)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Parameters</td>
<td>Values</td>
</tr>
<tr>
<td>Porosity, $n$</td>
<td>0.43</td>
</tr>
<tr>
<td>Molar mass of $Zn^{2+}$</td>
<td>0.065 kg m$^{-3}$</td>
</tr>
<tr>
<td>Molar mass of $Cd^{2+}$</td>
<td>0.112 kg m$^{-3}$</td>
</tr>
</tbody>
</table>
The initial and boundary conditions of the simulation are presented in Table 2 and the parameters in Table 3. The simulation results and their comparison with that of Do et al. (2006) are presented in Fig. 2. It is obvious from the graphs that the model predicted results agree well with the results of Do et al. (2006). The transport of Zn\textsuperscript{2+} and Cd\textsuperscript{2+} in these results are influenced by both the concentration gradients and the thermally induced diffusion or the Soret effect. The results also highlight accurate implementation of the mechanisms and its accuracy of prediction.

Figure 2 Comparison of model predicted concentration profiles of a) Zn\textsuperscript{2+} and b) Cd\textsuperscript{2+} against the results of Do et al. (2006).

4. Model applications

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soret Coefficient, $S_T$</td>
<td>0.033 K\textsuperscript{-1}</td>
<td>Hart and John (1986)</td>
</tr>
<tr>
<td>Diffusion coefficient ($D_0$) of Zn\textsuperscript{2+}</td>
<td>$7.02 \times 10^{-10}$ m\textsuperscript{2} s\textsuperscript{-1}</td>
<td>Lide (1997)</td>
</tr>
<tr>
<td>Diffusion coefficient ($D_0$) of Cd\textsuperscript{2+}</td>
<td>$7.17 \times 10^{-10}$ m\textsuperscript{2} s\textsuperscript{-1}</td>
<td>Lide (1997)</td>
</tr>
<tr>
<td>Distribution coefficient $K_d$ of Zn\textsuperscript{2+}</td>
<td>12.1 L kg\textsuperscript{-1}</td>
<td>Lin (2008)</td>
</tr>
<tr>
<td>Distribution coefficient $K_d$ of Cd\textsuperscript{2+}</td>
<td>26.8 L kg\textsuperscript{-1}</td>
<td>Lin (2008)</td>
</tr>
</tbody>
</table>
The model applications presented in this section investigate the relative importance of osmotic processes on non-isothermal coupled flow and deformation behaviour of a semi-permeable clay liner (bentonite) used in a generic landfill site.

4.1 Problem description

Waste weight and waste degradation, temperature evolution, leachate formation, and seepage create a complex, challenging scenario, for which optimum performance of the clay liner should be ensured and maintained to restrict the movement or spread of contaminants. Here, the model is used to simulate a number of coupled landfill processes in a 1D clay liner domain. Transport of a representative trace metal, e.g., Cadmium, is predicted in the saturated clay liner subjected to simultaneous thermal, chemical and mechanical loading events. Cadmium is a toxic heavy metal and causes adverse health consequences in human and animals when ingested at higher dosage.

Chen et al. (2015, 2016) reported that biological degradation of landfill waste can elevates the temperature at the top of the liner up to 80°C or 353 K, while the bottom temperature remains 20°C or 293 K. This creates a temperature gradient of 60°C across a 1.0 m long clay liner. In the simulations, three different temperatures, e.g. 313 K, 333 K and 353 K, have been considered at the top, while 293 K at the bottom, yielding $\Delta T = 20, 40$ and $60$, respectively. The simulation period is up to 100 years. The initial and boundary conditions of the simulations are presented in Table 4.

<table>
<thead>
<tr>
<th>Table 4</th>
<th>Initial and boundary conditions to investigate coupled THCM behaviour of a natural clay liner</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial conditions</td>
<td>Boundary conditions</td>
</tr>
<tr>
<td>$(0 &lt; z &lt; L)$</td>
<td>$(t &gt; 0)$</td>
</tr>
<tr>
<td>$w(z, 0)= 0$</td>
<td>$-$</td>
</tr>
</tbody>
</table>
\[ u(z, 0) = P = 50 \text{kPa} \quad u(0, t) = 0 \quad u(L, t) = 0 \]
\[ c(z, 0) = 0 \quad c(0, t) = 225 \quad c(L, t) = 0 \]
\[ T(z, 0) = 293 \text{K} \quad T(0, t) = 313 \text{K}/333 \text{K}/353 \text{K} \quad T(L, t) = 293 \text{K} \]

### 4.2 Model parameters

The model parameters are listed in Table 5. Gonçalvès and Trémosa (2010) compiled a list of thermo-osmotic conductivity data, from literatures, for various clays and expressed them in “m² K⁻¹ s⁻¹” unit by implicitly accounting the dynamic viscosity of water and osmotic efficiency of clayey soils. However, in these simulations the thermo-osmotic conductivity \((k_T)\) is calculated following Gonçalvès et al. (2012). This is because under non-isothermal condition \(\mu_t\) is a function of temperature \((T)\) and by considering it implicitly in m² K⁻¹ s⁻¹ units will undermine the important thermo-physical property of clay-water system. For boom clay, they reported the ratio of \(k_T/k\) in the range 2.5 - 250 Pa K⁻¹, where the intrinsic permeability \(k = 5.0 \times 10^{-18} \text{m}^2\). For \(k_T/k = 6.5 \text{ Pa K}^{-1}\), the value of \(k_T = 3.25 \times 10^{-17} \text{ Pa m}^2 \text{K}^{-1}\) or \(3.25 \times 10^{-17} \text{ N K}^{-1}\).

The temperature-dependent viscosity \(\mu_{t(T)}\) is estimated following (Kaye and Laby, 1986) as,

\[
\mu_{t(T)} = 661.2 (T - 229)^{-1.562} \times 10^{-3} \pm 0.5\% \quad (38)
\]

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Values</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial porosity, (n_0)</td>
<td>0.5</td>
<td></td>
</tr>
<tr>
<td>Molar mass of NaCl, (M)</td>
<td>0.112 kg mol⁻¹</td>
<td></td>
</tr>
<tr>
<td>Property</td>
<td>Value</td>
<td>Reference</td>
</tr>
<tr>
<td>----------------------------------------------</td>
<td>---------------------------</td>
<td>----------------------------------</td>
</tr>
<tr>
<td>Osmotic efficiency, $\omega$</td>
<td>0.005</td>
<td>Huang et al. (2015)</td>
</tr>
<tr>
<td>Density of the solid soil, $\rho_s$</td>
<td>2600 kg m$^{-3}$</td>
<td>Gonçalvès et al. (2012)</td>
</tr>
<tr>
<td>Diffusion coefficient ($D_0$) of Cd$^{2+}$</td>
<td>$3.837 \times 10^{-9}$ m$^2$ s$^{-1}$</td>
<td>Araujo et al. (2007)</td>
</tr>
<tr>
<td>Initial hydraulic conductivity, $k_0$</td>
<td>$1.0 \times 10^{-10}$ m s$^{-1}$</td>
<td>Kaczmarek et al. (1997)</td>
</tr>
<tr>
<td>Poisson’s ratio, $\nu$</td>
<td>0.3</td>
<td>Peters and Smith (2004)</td>
</tr>
<tr>
<td>Modulus of elasticity, $E$</td>
<td>$1.49 \times 10^6$ Pa$^{-1}$</td>
<td>Zhang et al. (2018)</td>
</tr>
<tr>
<td>Universal gas constant, $R$</td>
<td>8.314 J mol$^{-1}$ K$^{-1}$</td>
<td></td>
</tr>
<tr>
<td>Unit weight of the pore water, $\gamma_w$</td>
<td>10 kN m$^{-3}$</td>
<td></td>
</tr>
<tr>
<td>Distribution coefficient, $k_d$</td>
<td>$14.3 \times 10^{-3}$ m$^3$ kg$^{-1}$</td>
<td>Lin (2008)</td>
</tr>
<tr>
<td>Coefficient of volume change, $m_v$</td>
<td>$5 \times 10^{-7}$ Pa$^{-1}$</td>
<td>Delage et al. (2000)</td>
</tr>
<tr>
<td>Coefficient of volume change, $m_{\pi}$</td>
<td>$0.105 \times 10^{-7}$ Pa$^{-1}$</td>
<td>Kaczmarek and Hueckel (1998)</td>
</tr>
<tr>
<td>Soret coefficient, $S_T$</td>
<td>0.033 K$^{-1}$</td>
<td>Hart and John (1986)</td>
</tr>
<tr>
<td>Thermo-osmotic conductivity, $k_T$</td>
<td>$3.25 \times 10^{-17}$ Pa m$^2$ K$^{-1}$</td>
<td>Gonçalvès et al. (2012)</td>
</tr>
<tr>
<td>Thermal expansion coefficient, $\alpha$</td>
<td>$2.4 \times 10^{-4}$ K$^{-1}$</td>
<td>Hong et al. (2013)</td>
</tr>
<tr>
<td>Compressibility of pore fluid, $\beta_v$</td>
<td>$4.5 \times 10^{-10}$ Pa$^{-1}$</td>
<td>Francois et al. (2009)</td>
</tr>
<tr>
<td>Pore fluid thermal coefficient, $\beta_{fT}$</td>
<td>$3.5 \times 10^{-4}$ K$^{-1}$</td>
<td>Francois et al. (2009)</td>
</tr>
<tr>
<td>Specific heat capacity, $C_{ps}$</td>
<td>732 J kg$^{-1}$ K$^{-1}$</td>
<td>Francois et al. (2009)</td>
</tr>
<tr>
<td>Specific heat capacity, $C_{pf}$</td>
<td>4186 J kg$^{-1}$ K$^{-1}$</td>
<td>Francois et al. (2009)</td>
</tr>
<tr>
<td>Thermal conductivity of soil, $\lambda_T$</td>
<td>1.69 W m$^{-1}$ K$^{-1}$</td>
<td>Francois et al. (2009)</td>
</tr>
</tbody>
</table>

5. Results and Discussion

5.1 Effect of osmosis on the overall consolidation behaviour
The contributions of osmotic processes on the clay liner deformation are presented here. Various loading conditions including chemical-osmosis and thermo-osmosis are included in non-isothermal coupled flow simulations to estimate their relative dominance on the liner deformation. The results of four loading conditions, namely, Case 1: mechanical loading only; Case 2: mechanical loading and chemical-osmosis; Case 3: mechanical loading and thermo-osmosis; and Case 4: mechanical loading, chemical-osmosis and thermo-osmosis, at the source temperature of 333 K are presented in Fig.3. The deformation behaviour is explained by analysing the change in void ratio of the clay liner.

Fig.3a and 3b show the evolution of void ratio respectively at z = 0.25 m and 0.50 m for the four loading cases. In both figures, the lowest volume change is observed when the deformation is solely controlled by the mechanical loading, i.e. Case 1. The combination of mechanical loading, thermo-osmosis and chemical-osmosis (Case 4) results into the maximum deformation of the liner. The minimum void ratio observed in Fig.3a Case 1 and Case 4 are 0.94 and 0.86, while in Fig.3b these are 0.94 and 0.88, respectively. For the given simulation conditions and parameter regime, this represents an additional reduction of 8%, at 0.25 m depth, and 6%, at 0.50 m, of overall soil volume in Case 4 than in Case 1. In the simulation, liner temperature elevates rapidly and reaches to the applied temperature of 333 K at the boundary. The graphs of Case 3 as well Case 4, in both figures, indicate expansion of the clay liner during the temperature growth period (until around 0.01 years). This is related to the thermally induced expansions of soil skeleton and the pore fluid volume.
Figure 3: Evolution of void ratio and temperature at a) 0.25 m and b) 0.50 m depth of the semi-permeable clay liner for various loading situations. Case 1: mechanical loading only; Case 2: mechanical loading and chemical-osmosis; Case 3: mechanical loading and thermo-osmosis; and Case 4: mechanical loading, chemical-osmosis, and thermo-osmosis effects.

Following the initial expansion, pore fluid expulsion, assisted by the thermo-osmotic conductivity of the clay liner, occurs through the drainage boundary and causes thermo-osmotic consolidation. Closer
to the heat source the effect of thermo-osmotic consolidation and thermal consolidation is larger, which reduces gradually with the distance. This is noticeable, since the predicted slopes of Case 3 graphs in Fig.3a are steeper than that of Fig.3b.

The Case 2 graphs, which include the combined effects of mechanical loading and chemical-osmosis, show that initially the overall deformation is dominated by mechanical consolidation and in the long term chemico-osmotic consolidation becomes more prevalent. With time the gradient of solute concentration or chemical potential across the clay liner decreases and subsequently the effect of chemico-osmotic consolidation, which explains the ‘rebound shape’ observed in the Case 2 results. A detailed study on chemical-osmosis and chemico-osmotic consolidation behaviour of semi-permeable clays are presented in Zhang et al. (2018). It should be noted that under non-isothermal conditions temperature variations also influence the chemico-osmotic consolidation behaviours (as per Eq. (7)).
Figure 4 Evolution of solute concentration and temperature at (a) 0.25 m and (b) 0.50 m depth of the semi-permeable clay liner for various solute transport mechanisms. Case 1: chemical diffusion only; Case 2: thermal diffusion only; Case 3: fluid diffusion only; and Case 4: fluid diffusion, thermal diffusion, and chemical diffusion.

The calculated characteristic time \( \approx \frac{L^2}{D_c} \) for cadmium diffusion, for the parameter regime, are 2.05 years and 8.2 years at 0.25 m and 0.5 m, respectively. This is also noticeable in Figure 4a and 4b, which show the calculated results for the fluid diffusion, thermal diffusion, and chemical diffusion and combined actions in this consolidation problem. In comparison the characteristic times of thermal diffusivity, which is the ratio between thermal conductivity and specific heat capacity \( \approx 1.77 \times 10^{-6} \text{ m}^2/\text{s} \), for the corresponding characteristics length are significantly shorter, e.g., 9.8 hours and 39.2 hours. Based on the calculated coefficient of consolidation of \( 2.04 \times 10^{-8} \text{ m}^3/\text{s} \), the corresponding characteristic times for fluid diffusion are 35.4 days and 138.7 days. Therefore, the simulations suggest that the heat equilibrium reaches faster and before the pore water expulsion. The concentration equilibrium occurs at last. This means that the effects of heat transfer, fluid dissipation, and solute transport on the overall consolidation
of the liner occur perhaps independently.

5.2 Influence of temperature on the evolution and distribution of pore water

The evolution of excess pore water pressure along the depth of the clay liner is presented in Fig.5 for various temperature regimes. The results show that during the early simulation period (0.1 year), excess pore water pressure is positive and reaches near the applied mechanical pressure of 50 kPa. The positive porewater pressure (or compression) is associated with the mechanical consolidation and it increases further with temperature. This effect of temperature is repeated in each pressure profiles drawn at the individual simulation times, i.e. $t = 0.1, 1.0$ etc. However, the excess positive pressure disappears rapidly and leads to negative pressure development. The negative pressure in the clay liner occurs due to concurrent influence of chemical-osmosis and thermo-osmosis which expel pore water from the liner and results into negative pore water pressures. Therefore, under non-isothermal conditions, excess pore water pressure in semi-permeable clays is initially influenced by the mechanical loading and later combinedly by the osmotic loadings. The effects of osmotic consolidations on the excess pore water pressure gradually diminishes since both solute-concentration-gradient and temperature-gradient across semi-permeable clay membranes reduces with time.
Figure 5 Evolution and distribution of excess pore water pressure in the semi-permeable clay liner.

5.3 Influence of temperature on the overall liner settlement

The results of time-dependent settlement behaviour of the clay liner are presented Fig.6. The graphs plotted for the individual source temperatures exhibit an initial (I) increasing phase, followed by a (II) decreasing phase.
At lower temperatures, e.g. $\Delta T = 20^\circ C$, the contribution of thermally induced consolidation or expansion on the overall settlement is smaller and the settlement is dominated by the mechanical loading. The contributions of thermal volume change on the settlement increases with temperature, e.g. $\Delta T = 40^\circ C$ or $60^\circ C$. The graphs at these temperature regimes show an initial expansion of the liner that is due to the thermal dilation of the solid phase and the liquid phase. However, the differential expansion of the phases (liquid dilation is usually larger than a solid at a given temperature) leads to expulsion of pore water across the semi-permeable clay membrane under the drained boundary condition, i.e., thermo-osmotic consolidation. At higher temperature, the influence of thermo-osmotic consolidation on the overall settlement behaviour therefore increases. The peak settlement also increases with temperature. The maximum settlement of 27.55 mm is calculated at 353 K (or $\Delta T = 60^\circ C$), which is an increase of 11.3% from the peak settlement of 24.71 mm at the 313 K (or $\Delta T = 20^\circ C$). It is shown in Fig.3 that the mechanical consolidation occurs relatively fast and in the long-term both thermo-osmosis and chemical osmosis

**Figure 6** Evolution of the clay liner settlement for various temperature regimes.
influence the settlement behaviour. As the elevated thermo-osmotic-gradient and chemical-osmotic-gradient diminishes with time, the direction of pore water flow across the semi-permeable membrane reverses which leads to continuous reduction of the liner settlement. This explains the rebound shape observed in the phase II of Fig.6.

5.4 Influence of temperature and osmotic processes on the overall solute transport behaviour

The solute transport results in the clay liner is presented in Fig.7. In the simulations, a number of processes and their coupled interactions, including Fickian diffusion, temperature-induced diffusion or Soret effect, osmotically driven advection, chemico-osmotic consolidation, thermo-osmotic consolidation, mechanical consolidation and solid-solution partitioning or sorption, regulated the solute spread in the model domain. The results show that in semi-permeable clays solute spread is affected negatively with temperature, despite the influence of temperature on the solute movement (or the Soret effect) is positive. It is shown in Fig.6 that the liner settlement increases with temperature. That means that the solute transport is retarded further in a more compacted clay liner and, therefore, the effect of thermo-osmotic consolidation on the solute transport dominates over Soret diffusion. After 50 years, the concentration of 100 kg/m$^3$ Cd$^{2+}$ is predicted up to 0.12 m, 0.20 m, and 0.28 m depth, for $\Delta T = 20, 40, 60^\circ C$, respectively. For a 20°C increase in temperature the spread of cadmium in the liner is reduced by 8 cm for the current parameter regimes and the simulation conditions.

In practice, such as, landfill operations that often use clayey soils as barrier materials and where heat generation is significant, the effects of thermally driven consolidations should not be ignored, since it may significantly deviate the predicted outcomes. To highlight the importance of thermo-osmotic consolidation on solute transport, a comparison between hydro-mechanical-chemical (HMC) behaviour
and thermo-hydro-mechanical-chemical (THMC) behaviour of the clay liner is presented in Fig.8.

**Figure 7** Evolution of solute concentrations along the depth of the liner for various temperatures.

**Figure 8** Effect of temperature on solute transport behaviour in a saturated, semi-permeable clay liner.

THMC represents thermo-hydro-mechanical-chemical behaviour for non-isothermal simulation, whereas, HMC represent hydro-mechanical-chemical behaviour during isothermal simulations.

From the results of Fig.8, it is evident that significant difference exists between the THMC and the
HMC simulation. The solute concentration values in THMC simulations are less than those in HMC. Furthermore, the divergence between the THMC and the HMC simulation increases with time. In the HMC simulation, after 50 years, $Cd^{2+}$ concentration elevates to 50% of the source concentration level up to 0.16 m depth of the liner, whereas in the THMC simulation the spread is up to 0.109 m, which shows that the thermal mechanism has a great retardation effect on solute transport. That is an overprediction of 5.1 cm (31.9%) for a boundary temperature of 333 K (or $\Delta T = 40^\circ$C). In HMC simulation, thermo-osmotic consolidation and thermal diffusion are ignored, but the effects of mechanical loading, chemical-osmosis and other processes remain unchanged.

6. Conclusions

In this paper, a fully coupled numerical model to study thermo-hydro-mechanical-chemical behaviour of a saturated, semi-permeable clay soil, has been presented. The combined effect of thermo-osmosis and chemical-osmosis on soil deformation and solute transport behaviour has been investigated. Accuracy of the model in predicting the volume change behaviour and non-isothermal solute transport has been demonstrated via partial validation exercises supported by laboratory data collected from the literatures. In the application of the model, multiple loading events, e.g. mechanical loading, chemical loading, and thermal loadings are simultaneously imposed on a natural clay liner with the intention to identify the relative importance of thermo-osmotic consolidation on other loadings and to quantify its impact on the overall deformation of the liner as well as on the spread of a representative solute such as cadmium.

This study revealed that the effects of thermo-osmotic consolidation and the overall settlement of the clay liner increases with temperature. A change in temperature from 40$^\circ$C to 80$^\circ$C resulted in an
increase of 11.3% of the peak settlement (from 24.71 mm to 27.55 mm), for the same simulation period. At the early stages, soil settlement is dominated by the mechanical loading and, in the long-term, both chemico-osmotic consolidation and thermo-osmotic consolidation are found regulating the deformation behaviours. Excess porewater pressure in semi-permeable clays increases with temperature. Ignoring the thermo-osmosis and/thermo-osmotic consolidation processes in the simulations, the predicted transport significantly deviates from the realistic spread of the solute. Up to 80% overprediction of the spread of cadmium in the clay liner is observed when the thermo-osmotic processes are neglected.

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