Experimental and Numerical Investigation of Consolidation-Induced Solute Transport

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By

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ABSTRACT

Classical solutions for solute transport through a porous media are derived for rigid materials in which no deformation occurs during the transport process and advection is steady. There are cases, however, in which consolidation causes volume change during solute transport. The consolidation process takes on particular significance for fine grained soils at high water content, such as dredged sediments, but has also been shown to be important for compacted clay liners during waste filling operations.

A numerical model, called CST2, is presented for coupled large strain consolidation and solute transport in saturated porous media. The consolidation and solute transport algorithms include the capabilities of a previous code, CST1, with the addition of a variable effective diffusion coefficient during consolidation and nonlinear nonequilibrium sorption. A parametric study illustrates that, for the test cases considered, variation of effective diffusion coefficient during consolidation has an important effect on solute transport, and nonequilibrium (i.e., kinetic) sorption can have a
strong effect on consolidation-induced solute transport and that this effect becomes more
important as the rate of consolidation increases.

An experimental investigation was performed to determine the effect of clay
consolidation on solute transport parameters. In general, the experimental results
suggest that changes in effective diffusion and hydrodynamic dispersion coefficients
should be taken into account during clay consolidation whereas the sorption isotherm and
dispersivity may be considered as unchanged during the consolidation process.

Solute transport tests were conducted on composite specimens of kaolinite slurry
consisting of an upper uncontaminated layer and a lower layer contaminated with
potassium bromide. Numerical simulations were performed using the CST2 model.
The importance of the consolidation process on solute transport is assessed based on
measured and simulated solute breakthrough curves and final contaminant concentration
profiles. CST2 simulations closely match the experimental data for different initial
boundary and loading conditions. Results also indicate that both diffusion and
consolidation-induced advection made an important contribution to solute transport and
mass outflow, with consolidation having the largest effects for tracer transport. This study
suggests that neglecting transient consolidation effects may lead to significant errors in transport analyses involving soft contaminated clays undergoing large volume change.
To my parents, SunDal Lee and InSeang Kim

and my fiancée, Atsuko Maeda
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1.1 Background and Objectives

Consolidation-induced transport of contaminants occurs when contaminated soil undergoes consolidation due to changes in boundary stress conditions or material self-weight. The consolidation process takes on particular significance for fine grained soils at high water content, such as dredged sediments, but has also been shown to be important for compacted clay liners during waste filling operations (Peter and Smith 2002; Alshawabkeh and Rahbar 2006; Fox 2007b). Transport processes are similar to those for rigid porous media and include advection, dispersion, and sorption/desorption effects. The difference is that consolidation involves transient advective flows that are governed by the dissipation of excess pore pressures. These flows produce volumetric strains that, in turn, cause changes in soil compressibility and hydraulic conductivity. For small
strain conditions, such changes are neglected and associated transport analyses have been based on infinitesimal strain consolidation theory (Potter et al. 1994; Peter and Smith 1998; Alshawabkeh and Rahbar 2006). As strains increase, changes in compressibility and hydraulic conductivity can become large and transport analyses are treated within the context of large strain consolidation theory (Gibson et al. 1995; Peter and Smith 2002; Fox 2007a).

An example of a coupled consolidation–solute transport problem is the mechanical dewatering of contaminated, high water content, dredged sediment (Fox 2007a). The International Joint Commission (IJC), created by the United States and Canada to advise both governments on Great Lakes water issues, has designated 43 Areas of Concern (AOCs) in the Great Lakes region where the environment has been severely degraded. Contaminated sediments have been identified as a problem in 42 of these 43 AOCs. The most critical pollutants are polychlorinated biphenyls (PCBs) and other chlorinated compounds, polyaromatic hydrocarbons (PAHs), and metals (e.g., mercury, lead). These sediments are usually dredged instead of using in situ remediation methods because the wide variety of contaminants presents in each system. A large volume of dredged sediments with high moisture content can be dewatered by placement in a confined disposal facility as shown in Fig. 1.1. Several key questions arise for any such dewatering process (Fox 2007a): 1) What will be the amount and rate of pore water effluent? 2) What will be the concentration of contaminants in the effluent? 3) What will be the concentration and distribution of remaining contaminants in the dewatered
Solute transport models for rigid porous media are incapable of answering these questions because in this case advective flow is driven by the consolidation process.

Various numerical models have been developed to simulate solute transport within deforming porous media. In each case, the solute is considered to be sufficiently dilute that the problem can be treated as semi-coupled, with transient advective flows driving the transport process but solute concentrations not affecting media consolidation. Although large strains introduce significant changes in porosity, these models have assumed constant effective diffusion coefficient $D^*$ for simplicity.

Fig. 1.1  Aerial photo of confined disposal facility at Grand Calumet River in Gary after grading
Current models for consolidation-induced transport also assume linear equilibrium sorption (Peters and Smith 1998; Peters and Smith 2002; Alshawabkeh and Rahbar 2006; Fox 2007a). This assumption is potentially limiting from two standpoints. First, experimental evidence indicates that sorption is commonly nonlinear, particularly over large ranges of concentration, and is often characterized using the Langmuir and Freundlich isotherms (Travis and Etnier 1981). Second, equilibrium sorption is valid when advection is slow enough to provide sufficient reaction time between solute and soil solids. The early stages of consolidation can, however, involve very high rates of advection near drainage boundaries. As such, a nonequilibrium (kinetic) sorption model may be generally more suitable for simulations of consolidation-induced transport. The first objective of this research is to present the results of a numerical investigation of the significance of variable effective diffusion coefficient and nonlinear nonequilibrium sorption on consolidation-induced solute transport. Simulations were performed using a new numerical model CST2 (Consolidation Solute Transport 2), which is based on the code CST1 for coupled large strain consolidation and solute transport (Fox 2007a).

To provide input data for models of consolidation-induced transport, experimental investigations are needed to evaluate the effect of clay consolidation on solute transport parameters. Consolidation causes spatially and temporally varying void ratio, because applied surcharge pressure increases effective stress in deforming porous media. Accurate prediction of solute transport through the deforming porous media therefore requires a reliable estimation of the solute transport parameters for the conditions of changing void ratio. The second objective of this research is to present an experimental
investigation of the effect of clay consolidation on solute transport parameters such as effective diffusion coefficient, dispersivity, and sorption isotherm.

Most previous research on consolidation-induced solute transport has been performed using numerical models. A key shortcoming of this work is the absence of definitive experimental verification for these models. Some experimental research has been conducted using a geotechnical centrifuge (Potter et al. 1994, 1997; Moo-Young et al. 2001, 2003), and it was concluded that consolidation led to accelerated solute migration. Potter et al. (1997) showed that measured pore pressures and solute concentrations were in good to fair agreement, respectively, with numerical simulations obtained using a finite element model based on updated small strains. Moo-Young et al. (2003) did not compare simulations of consolidation-induced solute transport with the measured concentration data. Alshawabkeh et al. (2004) performed single-drained consolidation tests on composite kaolinite specimens consisting of two layers, and they concluded that consolidation accelerates solute transport if transient advective flows are in the same direction as the concentration gradient. However, comparison with numerical simulations was also not provided by Alshawabkeh et al. (2004). These studies have provided some insight into consolidation-induced solute transport. More definitive data is however needed for validation of computational models. The third objective of this dissertation is to present the results of a comprehensive experimental investigation of consolidation-induced solute transport and corresponding numerical simulations.
1.2 Dissertation Organization

This dissertation is organized as follows: Chapter 2 presents a literature review of past work related to the research topic. Chapter 3 presents the development of the CST2 numerical model including verification with existing analytical and numerical solutions, and a parametric study with respect to the significance of variable effective diffusion coefficient and nonlinear nonequilibrium sorption for consolidation-induced transport. Chapter 4 presents the experimental program used to evaluate the effect of clay consolidation on solute transport parameters and to investigate consolidation-induced solute transport. Chapter 5 presents the experimental results and numerical solutions for consolidation-induced solute transport for a variety of boundary conditions and loading schedules. Finally, Chapter 6 presents conclusions and recommendations for future research.
CHAPTER 2
LITERATURE REVIEW

This chapter reviews published research that is relevant to the topic of consolidation-induced solute transport. Most of this information is concerned with theoretical and numerical work. Less research has been published related to experimental investigations.

2.1 Solute Transport in Rigid Porous Media

The governing equation for one-dimensional solute transport in rigid porous media with sorption but excluding biological or chemical reactions is (Miller and Weber 1984),

\[
\frac{\partial c}{\partial t} + \left(1 - \frac{n}{n} \rho_s \right) \frac{\partial s}{\partial t} = D_h \frac{\partial^2 c}{\partial z^2} - v_s \frac{\partial c}{\partial z}
\]  

(2.1)
where \( c \) is dissolved solute concentration, \( t \) is time, \( z \) is the vertical coordinate taken as positive upward from the base of the specimen, \( n \) is total porosity, \( \rho_s \) is solid density, \( s \) is sorbed solute mass per mass of solid phase, \( D_h \) is the hydrodynamic dispersion coefficient, and \( v_s \) is the seepage velocity. The relative importance of advective transport based on \( v_s \) versus dispersive transport based on \( D_h \) is expressed using the Peclet number \( (P_L = \frac{v_s H}{D_h}) \), where \( H \) is specimen length. Shackelford (1994) states that advection governs solute transport for \( P_L \geq 50 \) and diffusion governs transport for \( P_L \leq 1 \). Gillham and Cherry (1982) found that diffusion is dominant when the seepage velocity is less than about \( 1.6 \times 10^{-10} \) m/s. For compacted clay liners, diffusion dominates the solute transport process due to the typically low advective flow rate (Crooks and Quigley 1984; Gillam et al. 1984; Rowe et al. 1988; Barone et al. 1989; Shackelford and Redmond 1995; Mazzieri et al. 2002).

Solute transport is mainly controlled by two parameters \( (D_h \) and \( v_s \)), and sorption in Eq. 2.1. These parameters and the sorption isotherm can be determined by back-calculation from experimental data obtained using soil column and batch tests or from field solute transport tests. A review of previous research related to each one is now presented.
2.1.1 Hydrodynamic dispersion coefficient

The process of hydrodynamic dispersion includes both diffusion and mechanical dispersion effects. The hydrodynamic dispersion coefficient ($D_h$) is defined as,

$$D_h = D^* + \alpha_L \gamma_s$$

(2.2)

where $D^*$ is the effective diffusion coefficient and $\alpha_L$ is the longitudinal dispersivity in the direction of transport. Due to tortuous flow pathways within a saturated soil, the effective diffusion coefficient is less than the free-solution diffusion coefficient ($D_o$). Therefore, $D^*$ is defined as $\tau_a D_o$, where $\tau_a$ is the apparent tortuosity factor of the medium. Several representative values of $D_o$ are listed in Table 2.1 for diffusion in free solutions at 25°C (Shackelford and Daniel 1991a).

Perkins and Johnson (1963) found that $\tau_a$ was equal to 0.7 for uniform sand. Gillham et al. (1984) studied the tortuosity for mixtures of bentonite and silica sand with non-reactive solutes ($^{36}$Cl and $^3$H) and found that the apparent tortuosity factor decreased as the clay content increased from 0 to 10% and then increased for mixtures having over 10% bentonite content (Table 2.2). At small clay contents, they proposed that the clay particles occupied the space between the sand grains and the lengths of the molecular pathways increased. As the clay content increased further, the effect of the sand grains decreased and path lengths decreased. Shackelford and Daniel (1991a, 1991b) reported $\tau_a$ values in the literature ranging from 0.01 to 0.84 for fine-grained soils and measured $\tau_a = 0.24$ to 0.53 for two compacted clays.
The value of $\tau_a$ is affected not only by pore space structure but also by physical-chemical interactions. Rowe et al. (1988) found that the result of physical-chemical interaction between Ca$^{2+}$ ions in solution and calcium rich clay of an unweathered gray clayey till increased the apparent tortuosity factor as compared to the same clay with a nonreactive tracer. Therefore, the effective diffusion coefficient of a specific soil can vary with particle structure and pore fluid chemistry.
<table>
<thead>
<tr>
<th>Anion</th>
<th>$D_o \times 10^{-10}$ (m$^2$/s)</th>
<th>Cation</th>
<th>$D_o \times 10^{-10}$ (m$^2$/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>OH$^-$</td>
<td>52.8</td>
<td>H$^+$</td>
<td>93.1</td>
</tr>
<tr>
<td>F$^-$</td>
<td>14.7</td>
<td>Li$^+$</td>
<td>10.3</td>
</tr>
<tr>
<td>Cl$^-$</td>
<td>20.3</td>
<td>Na$^+$</td>
<td>13.3</td>
</tr>
<tr>
<td>Br$^-$</td>
<td>20.8</td>
<td>K$^+$</td>
<td>19.6</td>
</tr>
<tr>
<td>I$^-$</td>
<td>20.4</td>
<td>Rb$^+$</td>
<td>20.7</td>
</tr>
<tr>
<td>HCO$_3$</td>
<td>11.8</td>
<td>Cs$^+$</td>
<td>20.5</td>
</tr>
<tr>
<td>SO$_4$$^{2-}$</td>
<td>10.6</td>
<td>Be$^{2+}$</td>
<td>5.98</td>
</tr>
<tr>
<td>CO$_3$$^{2-}$</td>
<td>9.22</td>
<td>Mg$^{2+}$</td>
<td>7.05</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Ca$^{2+}$</td>
<td>7.92</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Sr$^{2+}$</td>
<td>7.90</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Ba$^{2+}$</td>
<td>8.46</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Pb$^{2+}$</td>
<td>9.25</td>
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<td></td>
<td></td>
<td>Cu$^{2+}$</td>
<td>7.13</td>
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<td></td>
<td></td>
<td>Fe$^{2+}$</td>
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</tr>
<tr>
<td></td>
<td></td>
<td>Cd$^{2+}$</td>
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<td></td>
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<td>Zn$^{2+}$</td>
<td>7.02</td>
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<td>Ni$^{2+}$</td>
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<td></td>
<td>Fe$^{3+}$</td>
<td>6.07</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Cr$^{3+}$</td>
<td>5.94</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Al$^{3+}$</td>
<td>5.95</td>
</tr>
</tbody>
</table>

Table 2.1  Self-diffusion coefficients for representative ions at infinite dilution in water at 25°C (Shackelford and Daniel 1991a)
<table>
<thead>
<tr>
<th>Bentonite Content (%)</th>
<th>Apparent Tortuosity Factor ($\tau_a$)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Chlorine-36 ($^{36}$Cl)</td>
</tr>
<tr>
<td>0</td>
<td>0.84</td>
</tr>
<tr>
<td>5</td>
<td>0.67</td>
</tr>
<tr>
<td>10</td>
<td>0.59</td>
</tr>
<tr>
<td>15</td>
<td>0.67</td>
</tr>
<tr>
<td>25</td>
<td>0.67</td>
</tr>
<tr>
<td>50</td>
<td>0.76</td>
</tr>
<tr>
<td>100</td>
<td>0.84</td>
</tr>
</tbody>
</table>

Table 2.2  Apparent tortuosity factor for the non-reactive solutes $^{36}$Cl and $^3$H (Gillham et al. 1984)

Mechanical dispersion is the mixing of a solute due to variations of pore-scale flow velocity and can be quantified in the longitudinal direction as $\alpha_v v_z$ (Eq. 2.2). Many researchers have measured values of mechanical dispersion for various levels of heterogeneity in natural soils and found that the dispersivity ($\alpha_z$) is significantly dependent on the representative length scale. This occurs because, as the length scale increases, the flow domain unavoidably includes progressively larger scale
heterogeneities. Gillham and Cherry (1982) found that $\alpha_L$ values determined in the laboratory (usually for tracers) generally range from 0.1 to 10 mm and Fried (1972) suggested 1 mm as an average value. Taylor et al (1987) found that $\alpha_L$ values from laboratory tests were generally an order of magnitude lower than values from field tests. This is consistent with Lallemand-Barres and Peaudecerf (1978), who proposed a “one-tenth rule” which defines dispersivity as equal to one-tenth of the distance traveled by the solute, and the EPA (1985) has recommended this method to estimate dispersivity for cases in which no data exists. However, Gelhar et al. (1992) commented that the “one-tenth rule” is not accurate due to differing degrees of aquifer heterogeneity at different sites. Field tracer tests remain the best method to measure macroscopic dispersivity in order to predict solute transport at field scale, but these tests are costly and time consuming and as a result are rarely performed.

2.1.2 Seepage velocity

The movement of contaminants with flowing pore water (advective transport) is mainly controlled by seepage velocity ($v_s = \frac{v}{n_{eff}}$), where $v$ ($= ki$) is the discharge velocity, $n_{eff}$ is effective porosity, $k$ is the hydraulic conductivity, and $i$ is the hydraulic gradient. Effective porosity is the fraction of soil volume that conducts flow and, therefore, excludes dead end pores and small channels that do not participate in the transport process. For granular soils, $n_{eff}$ is essentially equal to total porosity $n$. However, $n_{eff}$ can be substantially less than $n$ for clayey soils. The value of $n_{eff}/n$
can be expected to range from 0.25 to 1.0 (Edil 2003). Rowe et al. (1988) conducted column tests for saturated Sarnia till. From measured parameters at different porosities, they concluded that the effective porosity was not significantly less than the total porosity. Kim et al. (1997) found that the effective porosity was equal to 89 to 104% of the total porosity. However, considering the measurement error for total porosity and the uncertainty in measuring and back-calculating effective porosity, they concluded that the effective porosity was essentially the same as the total porosity for Kirby Lake till.

2.1.3 Sorption

In general, a sorption isotherm is nonlinear and time-dependent (van Genuchten and Wagenet 1989). Nonequilibrium sorption may be important during a column test with a fast advection rate because the system may not have sufficient time to come to equilibrium (Wu and Gschwend 1986). The general case corresponds to the following nonlinear nonequilibrium (i.e., kinetic) sorption model (Travis and Etnier 1981):

\[
\frac{\partial s}{\partial t} = \lambda (K_p c^F - s)
\]  

(2.3)

where \( \lambda \) is a kinetic rate constant, and \( K_p \) and \( F \) are constants describing the nonlinear Freundlich isotherm. The rate of solute mass transfer is controlled by the imbalance of concentrations with respect to equilibrium, which is defined as

\[
s = K_p c^F
\]  

(2.4)

Conceptually, equilibrium sorption can be achieved using Eq. 2.3 as \( \lambda \rightarrow \infty \). When the Freundlich isotherm is linear \( (F = 1) \), \( K_p \) is called the equilibrium sorption
distribution coefficient \( (K_d) \) which is the slope of a linear sorption isotherm that passes through the origin. The distribution coefficient is often used because the governing equation (Eq. 2.1), which assumes linear sorption, is relatively easy to solve mathematically.

2.1.4 Column test analysis

Solutions to Eq. 2.1 can be used to evaluate spatial and temporal variations in solute concentration within a rigid porous medium, but concentration boundary conditions must be specified carefully. For example, laboratory soil column tests are assumed to be performed with an initially uncontaminated specimen. A contaminated solution with constant concentration is injected into the soil at a constant flow rate. Effluent water samples are collected at the other end of the column and concentration changes are measured as a function of time, which is called a “breakthrough curve”. The breakthrough curve is often used to estimate solute transport parameters due to the relative ease of measuring concentrations at the effluent boundary as compared to concentrations inside the column (Shackelford 1994).

Analytical solutions and numerical models can be used to calculate dispersion and sorption transport parameters from experimental breakthrough curves. These methods vary with regard to choice of concentration variable, initial and boundary conditions, and linearity of sorption isotherm. Breakthrough curves from the dispersion column tests can be analyzed using three methods that differ with regard to choice of concentration variable and outflow (top) boundary condition (van Genuchten and Parker 1984).
inflow (bottom) boundary is characterized using a prescribed mass flux condition in each case. Method I is defined in terms of resident concentration for a semi-infinite column, which gives the following boundary conditions,

\[ v_s c_o = v_s c_r - D_h \frac{\partial c_r}{\partial z} \quad \text{at } z = 0 \quad (2.5) \]

\[ \frac{\partial c_r}{\partial z} = 0 \quad \text{at } z = \infty \quad (2.6) \]

where \( c_r \) is resident (i.e., dissolved) solute concentration in the pore fluid. Method II uses flux-averaged concentration \( c_f \) (Kreft and Zuber 1978),

\[ c_f = c_r - \left( \frac{D_h}{v_s} \right) \left( \frac{\partial c_r}{\partial z} \right) \quad (2.7) \]

and a semi-infinite outflow boundary condition,

\[ \frac{\partial c_f}{\partial z} = 0 \quad \text{at } z = \infty \quad (2.8) \]

Substituting (2.7) into (2.5), the inflow boundary condition for Method II simplifies to a constant flux-averaged concentration (i.e., \( c_f = c_o \) at \( z = 0 \)). Method III is defined in terms of resident concentration, finite specimen length, and a zero-gradient the outflow boundary condition. This gives the following boundary conditions,

\[ v_s c_o = v_s c_r - D_h \frac{\partial c_r}{\partial z} \quad \text{at } z = 0 \quad (2.9) \]

\[ \frac{\partial c_r}{\partial z} = 0 \quad \text{at } z = H \quad (2.10) \]
Most previous researchers have recommended Method II for the analysis of measured breakthrough curves from dispersion column tests (van Genuchten and Parker 1984; Parker 1984; Shackelford 1994). Those studies were focused on transport of nonreactive tracers and solutes with a linear sorption isotherm. No comparative studies have been reported for cases involving nonlinear sorption.

2.1.5 Conclusion

Eq. 2.1 is derived assuming that porosity is constant and seepage velocity is uniform - in other words, steady flow through a rigid porous medium. However, significant volumetric strains may occur during the transport process. Examples include dewatering of contaminated soil or waste materials, simultaneous consolidation and solute transport through compacted clay liners, and consolidation of contaminated clay deposits. The assumption of rigid porous media is not valid in such cases because media consolidation due to an increase in effective stress causes spatial and temporal changes in void ratio. Before discussing solute transport in a deforming media, it is necessary to first review theories of one-dimensional consolidation for both small strain and large strain conditions.

2.2 Consolidation Theory

Consolidation is the process by which the volume of a saturated soil decreases due to the dissipation of excess pore pressure. In the case of one-dimensional loading, the applied stress increment is initially transferred almost completely to the pore water.
With time, water flows out of the soil and the pore water pressure decreases. Concurrently, soil volume decreases as there is a gradual transfer of stress from the pore water to the soil skeleton, which is called effective stress. Finally, the soil skeleton supports the applied stress and the excess pore water pressure (i.e., the fraction of total pore pressure that is due to the loading) is fully dissipated. Thereafter, small reductions of soil volume are still possible due to secondary compression, which is not considered as part of the consolidation process.

2.2.1 Small strain consolidation theory

The Terzaghi one-dimensional consolidation theory (Terzaghi 1925) is widely used for settlement analysis in geotechnical engineering. This theory was developed based on the following assumptions: 1) the soil is homogeneous and 100% saturated, 2) drainage is provided at one or both boundaries of the compressible layer, 3) Darcy’s law is valid, 4) the law of effective stress is valid, 5) the soil particles and water are incompressible, 6) compression and flow are one dimensional, 7) there is an unique linear relationship between void ratio ($e$) and vertical effective stress ($\sigma'_v$), and 8) changes in thickness of the layer sufficiently are so small that they can be neglected. It is this later assumption that relegates Terzaghi theory as a small strain theory. Therefore, not only do compressibility and hydraulic conductivity remain constant during the consolidation process, but also the layer thickness is assumed to be constant. Also, the stresses from the self-weight of the layer are assumed to be negligible. As a result, Terzaghi theory is more directly applicable to thin layers.
For a thick clay layer with high moisture content, however, the applied load increment may cause large strains, which often results in a nonlinear $e - \sigma'_v$ relationship and variable hydraulic conductivity during the consolidation process. The self-weight of the soil skeleton and the pore water should be considered for such cases (Gibson et al. 1981; Cargill 1984). Olson and Ladd (1979) concluded that significant errors of classical analyses may occur when the stress-strain relationship is highly nonlinear. McVay et al. (1986) described that, in case of waste containment ponds, the hydraulic conductivity may vary over several orders of magnitudes and the soil skeleton may undergo volumetric strains of 50% or more.

2.2.2 Theories for large strain consolidation

Large strain consolidation theory removes the limitation of small strains and can accommodate changes in compressibility and hydraulic conductivity during the consolidation process (Gibson et al. 1967). In addition, the self-weight of the soil layer can be included (Gibson et al. 1981). The derivation of the governing equation for large strain consolidation theory is now reviewed.

One of the first key differences with small strain consolidation theory is the consideration of coordinate system. Various theories of large strain consolidation have been developed using different coordinate systems. The usual coordinate system in geotechnical engineering is the spatial (Eulerian) coordinate where material deformation is related to planes that are fixed in space for all time. For small deformations, the thickness of a compressible soil layer is assumed to remain constant and the distance
from an arbitrary datum to any representative elementary volume (REV) is also constant. For large deformations, however, the REV moves in space and does not remain at the same position. For example, assume a piezometer is placed a small distance below the top-drained boundary of a highly compressible soil. The soil experiences a large settlement over some time increment, so the piezometer is eventually outside of the layer according to a spatial coordinate system. However, a real piezometer would move with the soil and always measure pore water pressure of the same material point as a function of time (Gibson et al. 1981).

A material (Lagrangian) coordinate system refers all quantities to the initial configuration of the layer \((t = 0)\). As shown in Fig. 2.1, the position of the upper boundary remains at \(a = 0\) for any time \(t\), where \(a\) is the Lagrangian coordinate (positive in the direction of gravity). The main issue then becomes how to trace the real position of a material point if the upper and lower boundaries always remain \(a = 0\) and \(a = H_o\), where \(H_o\) is the initial height of the soil layer. A new distance \(\xi\) is defined to locate each material point as a function of time. At any time, the real position of a material point is converted with (Fig. 2.1(b))

\[
\xi(a,t) = a + S(a,t) \tag{2.11}
\]

where \(S\) is the settlement. With time, for instance, the real position of upper boundary \((a = 0)\) moves with the settlement of the soil \((\xi(0,t) = S(0,t))\). The upper boundary condition expressed in terms of material coordinates is a dependent variable of the unknown surface settlement \(S(0,t)\), so the solution process is not straightforward (Xie and Leo 2004). From a physical view point, however, it is convenient to derive the
Consider that a REV having unit cross-sectional area is initially located in space between the points $a$ and $a + da$ in a material (Lagrangian) coordinate system. At any time $t$, the REV settles and is located in the space between the points $\xi$ and $\xi + d\xi$ measured relative to an embedded datum plane at $\xi = 0$. During consolidation, pore fluid is squeezed from the REV, but the solid phase remains in the REV.

Fig 2.1. Lagrangian coordinates: (a) initial configuration at $t = 0$, and (b) current configuration at $t > 0$ of a consolidating layer (Xie and Leo 2004).
The consolidation equation can be derived from conservation of mass of incompressible water and solid phases (Eq. 2.12 and 2.13), and Darcy’s law (Eq. 2.14). By using material (Lagrangian) coordinates, these relationships are given by (Peters and Smith 2002),

\[
\frac{\partial (\nu)}{\partial a} = \frac{\partial}{\partial t} \left( n \frac{\partial \xi}{\partial a} \right) \quad (2.12)
\]

\[
\rho_s (a,0)(1-n_o) = \rho_s (1-n) \frac{\partial \xi}{\partial a},
\]

therefore

\[
\frac{\partial \xi}{\partial a} = \frac{1-n_o}{1-n} = \frac{1+e}{1+e_o} \quad (2.13)
\]

\[
v = -\frac{k}{\gamma_w} \left( \frac{\partial u_e}{\partial \xi} \right) \quad (2.14)
\]

where \( n_o \) is initial porosity, \( k \) is vertical hydraulic conductivity, \( \gamma_w \) is unit weight of water, and \( u_e \) is excess pore water pressure. Constitutive relationships for \( \sigma'_v \) and \( k \) are expressed explicitly in terms of the void ratio as

\[
\sigma'_v = f(e)
\]

and \( k = f(e) \quad (2.15) \)

By substituting Eqs. 2.13 and 2.14 into Eq. 2.12, and then applying \( \sigma'_v = \sigma_v - (u_s + u_e) \) where \( \sigma_v \) is vertical total stress, \( u_s \) is hydrostatic pore water pressure, the consolidation equation is (McVay et al. 1986, 1989)

\[
\frac{\partial}{\partial \xi} \left( \frac{k}{\gamma_w} \frac{\partial u_e}{\partial \xi} \right) = -\frac{1}{1+e} \frac{de}{dt} \frac{\partial u_e}{\partial \sigma'_v} \quad (2.16)
\]
Lee and Sills (1979) developed a similar one-dimensional consolidation equation using a spatial (Eulerian) coordinate system and a moving boundary approach.

For small strains, 1) hydraulic conductivity is assumed to be independent of spatial position,

\[
\frac{\partial}{\partial \xi} \left( k \frac{\partial u_e}{\partial \xi} \right) \Rightarrow \frac{k}{\gamma_w} \frac{\partial^2 u_e}{\partial \xi^2}
\]  

and 2) the stress-strain relationship is assumed to be linear,

\[
\frac{de}{d\sigma'_v} = -a_v
\]  

where \( a_v \) is coefficient of compressibility. Eq. 2.16 then simplifies to the classical Terzaghi consolidation equation,

\[
\frac{k}{\gamma_w} \frac{\partial^2 u_e}{\partial \xi^2} = a_v \frac{\partial u_e}{\partial t}
\]

or

\[
\frac{\partial u_e}{\partial t} = c_v \frac{\partial^2 u_e}{\partial \xi^2}
\]  

where \( c_v = \left( k(1+e) / a_v \gamma_w \right) \) is the coefficient of consolidation.

A third coordinate system, called a reduced coordinate system, consists of the independent variables \( w \) and \( t \), where \( w \) represents the volume of soil particles between the datum plane and the point of interest. Even though the solid surface is settling downward, its reduced coordinate position is unchanged (Fig 2.2).
Fig 2.2 Phase diagrams for (a) initial and (b) current configuration of material element of soil (Lehner 1984).

Gibson et al. (1967) proposed a large strain consolidation theory in reduced coordinates, which has been widely used in numerical models (McVay et al. 1986; Townsend and McVay 1990). The material (Lagrangian) coordinate system can be transformed to a reduced coordinate system using the chain rule as

\[
\frac{\partial f}{\partial w} = \frac{\partial f}{\partial \xi} \frac{\partial \xi}{\partial w} + \frac{\partial f}{\partial t} \frac{\partial t}{\partial w}
\]  

(2.20)
where \( f \) is an arbitrary function of \( \xi \) and \( t \), and \( \frac{\partial t}{\partial w} = 0 \) because \( w \) and \( t \) are independent variables. Eq. 2.16 can be converted into reduced coordinates \((w,t)\) by using Eq. 2.20, and the partial derivative \( \frac{\partial \xi}{\partial w} \) may be evaluated as (Fig. 2.2),

\[
\frac{\partial \xi(w,t)}{\partial w} = 1 + e(w,t) \tag{2.21}
\]

The derivative of excess pore water pressure is expressed using buoyant unit weight and effective stress (McVay et al. 1986) as,

\[
\frac{\partial u^e}{\partial w} = (\gamma_s - \gamma_w) - \frac{\partial \sigma'_v}{\partial w} \tag{2.22}
\]

where \( \gamma_s \) is the unit weight of solids. If Eq. 2.22 is substituted into Eq. 2.16 with void ratio as the dependent variable (instead of excess pore pressure), one obtains (Gibson et al. 1967),

\[
-\left(\frac{\gamma_s}{\gamma_w} - 1\right) \frac{d}{de} \left[ \frac{k}{1+e} \frac{\partial e}{\partial w} + \frac{\partial}{\partial w} \left[ \frac{k}{\gamma_w (1+e)} \frac{d\sigma'_v}{de} \frac{\partial e}{\partial w} \right] + \frac{\partial e}{\partial t} \right] = 0 \tag{2.23}
\]

This is a general equation for one-dimensional large strain consolidation in a reduced coordinate system. The first term of Eq 2.23 accounts for self weight consolidation of a thick layer and second term results from external forces acting on the soil layer (Peters and Smith 2002).

Yong et al. (1983) applied piecewise-linear analysis to solve the large strain consolidation problem. Yong and Ludwig (1984) developed the same one-dimensional consolidation equation (Eq 2.16), and solved it using a piecewise-linear approach in which all variables pertaining to problem geometry, material properties, fluid flow and
effective stress are updated after each time step with respect to a fixed Eulerian coordinate system. Fig. 2.3 shows the computational flow chart for the model. The piecewise-linear approach is generally considered to have greater versatility with regard to initial conditions, boundary conditions, and soil heterogeneity than models based on material coordinates (Townsend and McVay 1990). Fox and Berles (1997) presented a piecewise-linear numerical model for one-dimensional consolidation called CS2 (Consolidation Settlement 2). The comparatively simple formulation of CS2 makes it particularly advantageous for the incorporation of additional modifications, including layered systems, time-dependent applied loads and piezometric groundwater levels, depth-dependent and pre-existing initial excess pore pressures, log-linear constitutive relationships including a preconsolidation pressure and unloading/reloading effects. Solid mass conservation can be strictly enforced and, as such, the method is actually a Lagrangian approach that follows the motion of the solid phase throughout the consolidation process.
Fig. 2.3 Computational method of Yong’s piecewise-linear model (Yong and Ludwig 1984).
The method has proven reliable with the ability to accommodate accreting layers (Fox 2000), radial flow to vertical drains (Fox et al. 2003), compressible pore fluid (Fox and Qiu 2004), high-gravity conditions in a geotechnical centrifuge (Fox et al. 2005; Lee and Fox 2005), and, when inertial effects are included, wave propagation in saturated porous media (Qiu and Fox 2007). Brief summary of the CS2 model is presented here.

The initial geometry of the soil specimen at the beginning of consolidation \( t = 0 \) is shown in Fig. 2.4(a). Friction against the sides of the specimen is neglected such that the specimen can be treated as a one-dimensional column. The soil is assumed to be an idealized two-phase homogenous material in which both the soil particles and pore fluid are incompressible. Vertical coordinate \( z \) and element coordinate \( j \) are defined as positive upward from a fixed datum plane at the base of the specimen. The column is divided into \( R_j \) elements, each \( j^{th} \) element having unit cross sectional area, initial height \( L_o \), a central node located at initial elevation \( z_{o,j} \), and initial void ratio \( e_{o,j} \). The top and bottom boundaries of the specimen can be specified as drained or impermeable. Drained boundaries are hydraulically connected to a groundwater table (i.e., surface of zero pore pressure) at constant elevation \( H_w \) above the datum. At \( t = 0 \), an instantaneous vertical effective stress increment, \( \Delta q \), is applied to the compressible stratum. Thereafter, both \( q_o \) and \( \Delta q \) are constant and move with the upper boundary. The geometry of the column at some later time is shown in Fig. 2.4(b). The height of the specimen is \( H' \), the height of the \( j^{th} \) element is \( L'_j \). Excess pore pressures cause fluid flow from the interior of the column to all drainage boundaries. Soil deformation
occurs in response to the net fluid outflow from each element. Node positions remain at the center of their respective elements throughout the consolidation process and are updated at each time step.

Constitutive relationships for the soil, shown in Fig. 2.5, are specified using discrete data points. The compressibility curve (Fig. 2.5a) is defined by $R_m$ ($\geq 2$) pairs of corresponding effective stress $\hat{\sigma}'$ and void ratio $\hat{e}$. The hydraulic conductivity relationship (Fig. 2.5b) is defined by $R_n$ ($\geq 2$) pairs of corresponding void ratio $\bar{e}$ and hydraulic conductivity $\bar{k}$. An element becomes overconsolidated if the effective stress decreases below the preconsolidation stress $\sigma''_{p,j}$ (i.e., maximum past effective stress) for the element. In this case, unloading and reloading follow an identical path defined by $\sigma''_{p,j}$, the corresponding preconsolidation void ratio $e'_{p,j}$, and a constant recompression index $C_r = \Delta e / \Delta \log_{10} \sigma'$. 


Fig. 2.4  Geometry for CS2:  (a) initial condition ($t = 0$) and (b) configuration at some later time $t$. 
The constitutive relationships can, overconsolidated conditions, which is consistent with the findings of Al-Tabbaa and CS2 uses the same hydraulic conductivity relationship for normally consolidated and does not account for the effects of strain rate, secondary compression, or aging on the compressibility or hydraulic conductivity of the soil. The constitutive relationships can,

CS2 uses the same hydraulic conductivity relationship for normally consolidated and overconsolidated conditions, which is consistent with the findings of Al-Tabbaa and Wood (1987), Nagaraj et al. (1994), and Fox (2007b). Aside from unload/reload effects, a one-to-one correspondence is assumed for each constitutive relationship. Thus, CS2 does not account for the effects of strain rate, secondary compression, or aging on the compressibility or hydraulic conductivity of the soil. The constitutive relationships can,
however, take essentially any desired form by choosing the appropriate number of data points.

Total stress at the $j^{th}$ node at time $t$, $\sigma_j^t$, is computed from overburden pressure and the self-weight of overlying elements,

$$\sigma_j^t = H_w - H^t + q_o + \Delta q + \frac{L_j \gamma_j^t}{2} + \sum_{i=j+1}^{R_j} L_i \gamma_i^t \quad j = 1, 2, ..., R_j \quad (2.24)$$

where $\gamma_j^t$ is the saturated unit weight of element $j$. Effective stress at the $j^{th}$ node $\sigma_j'^t$ is computed from $e_j^t$ and the compressibility curve (Fig. 2.5a). The pore pressure at the $j^{th}$ node $u_j^t$ is the difference between the total and effective stresses ($u_j^t = \sigma_j^t - \sigma_j'^t$), and $u_j^t$ with $j^{th}$ element elevation ($z_j^t$) is used to calculate total head.

Flow between adjacent elements is computed using the Darcy-Gersevanov law (Schiffman et al. 1985) which accounts for the relative motion of fluid and solid phases. The relative discharge velocity $v_{sf,j}^t$ between nodes $j$ and $j+1$ is $v_{sf,j}^t = -k_{s,j}^t i_j^t$, where $k_{s,j}^t$ is the equivalent series hydraulic conductivity between nodes $j$ and $j+1$, and $i_j^t$ is hydraulic conductivity between adjacent elements, which is calculated with total heads and node elevations of the adjacent elements (Fox and Berles 1997). CS2 performs a search over all elements at each time step to find the smallest value of $\Delta t$, which is then used to advance the solution forward in time for all elements. Once the discharge velocities and time incremental ($\Delta t$) are known, new element heights are calculated and
new void ratios are updated. After the new height of the specimen \(H^{t+\Delta t}\) is calculated, updated settlement \(S^{t+\Delta t}\) is,

\[
S^{t+\Delta t} = H_0 - H^{t+\Delta t}
\]  

(2.25)

The above method precisely conserves solid mass within each element throughout the consolidation process (Fox and Berles 1997). Thus, the method follows the motion of the solid phase and solid mass does not cross element boundaries.
2.2.3 Conclusion

Currently available models for large strain consolidation employ a number of numerical approaches involving different independent variables and coordinate systems, including the piecewise-linear method. If done correctly, the results of these models will not show significant differences because the governing equations follow the same basic laws; continuity of solids and fluids, balance of momentum, and constitutive relationships. McVay et al. (1986) concluded that different available models to solve Eq. 2.16 and Eq. 2.23 show identical excess pore pressure, void ratio, and settlement predictions. Fox and Berles (1997) compared the computed settlement versus time curve and void ratio distribution obtained using CS2 with the numerical simulations of McVay et al. (1986). As shown in Fig. 2.6(a) and 2.6(b), the values are in excellent agreement for each plot.
Fig. 2.6  Comparison of numerical models; (a) settlement vs. time and (b) void ratio distribution (Fox and Berles 1997)
2.3 Coupled Large Strain Consolidation and Solute Transport

Several research groups have turned their attention to the modeling of consolidation-induced solute transport. Most previous works have been conducted within the context of infinitesimal strain consolidation theory (Potter et al. 1994; Loroy et al. 1996; Smith 1997; Peters and Smith 1998; Van Impe et al. 2002; Alshawabkeh et al. 2005; Alshawabkeh and Rahbar 2006). Gibson et al. (1995) were the first to discuss coupled solute transport within the context of large strain consolidation theory. Their theoretical development is presented without solution and addresses various coordinate references frames, boundary conditions, and dependent variables for the transport of a single tracer (i.e., non-sorbing) solute. Smith (2000) expanded the Smith (1997) small strain model to include nonlinear large strain theory and presented analytical solutions for a quasi-steady-state small strain transport problem. Peters and Smith (2002) extended further the Smith (2000) theory to consider time-dependent solute transport through a deforming porous medium in both spatial (Eulerian) and material (Lagrangian) coordinates.

The piecewise-linear numerical approach for the prediction of large strain consolidation is generally considered to have greater versatility than models based on material coordinates. CS2 (Fox and Berles, 1997) is currently the leading piecewise-linear model. The framework for CS2 is particularly well suited for the incorporation of additional modifications and has proven to be both reliable and robust in subsequent studies. A new approach for the simulation of coupled nonlinear large strain consolidation and solute transport is based on the piecewise-linear method and is coded
in the numerical model CST1 (Fox 2007a). A complete review of the formulation and capabilities of CST1 is provided by Fox (2007a), and brief summary is provided herein. The consolidation algorithm like CS2 is one-dimensional and accounts for vertical strain, soil self-weight, general constitutive relations, relative velocity of fluid and solid phases, changing hydraulic conductivity and compressibility during consolidation, time-dependent loading, unload/reload effects, and an external hydraulic gradient acting across the layer. Constitutive relationships for the soil are defined using discrete data points and can take nearly any desired form. The solute transport algorithm of CST1 is two-dimensional and accounts for advection, longitudinal and transverse dispersion, first-order decay reactions, and linear equilibrium sorption. Solute transport is consistent with temporal and spatial variations of porosity and seepage velocity in the consolidating layer. The key to the transport model is the definition of two Lagrangian fields of elements that follow the motions of fluid and solid phases separately as shown in Fig. 2.7.

2.3.1 Geometry

While the movement of all soil particles and pore fluid occurs exclusively in the vertical direction, the layer is represented as two-dimensional to accommodate both longitudinal (vertical) and transverse (horizontal) hydrodynamic dispersion processes. Fluid and solid elements move independently except that they are coupled via values of solid element-to-solid element relative discharge velocity that govern the movement of each system. This dual-Lagrangian analysis framework follows the motions of fluid and solid phases separately and thereby avoids numerical dispersion that occurs if advection-
dispersion transport is calculated using a single field of well-mixed solid elements (Fox 2007a). A time-dependent vertical effective stress increment $\Delta q'$ is applied to the layer beginning at time $t = 0$ and moves with the top boundary thereafter. Excess pore pressures created as a result of the stress increment cause fluid flow from the interior of the soil layer to all drainage boundaries like CS2. Soil deformation occurs in response to the net fluid outflow from each solid element. Solute transport occurs by advection and dispersion in the fluid phase and sorption onto moving solid elements.

The configuration of the system at some later time $t$ is shown in Fig. 2.7(b). Fluid and solid elements have been laterally separated for clarity but, similar to Fig. 2.7(a), occupy the same physical space. Fluid elements maintain their original horizontal positions but become vertically disconnected from their original solid elements and move in response to the seepage velocity field. Fluid elements always contain their original fluid volume unless they are adjacent to a drainage boundary. Thus, for problems involving consolidation (as opposed to swelling), the heights of fluid elements will increase as the porosity of the associated solid elements decreases. Fluid elements move through, and possibly out of, the consolidating layer in response to excess pore pressures and any external hydraulic gradient (if $h_i \neq h_b$, where $h_i$ and $h_b$ are total head at top and bottom boundary, respectively). Thus, unlike the number of solid elements which is always constant, the number of fluid elements may decrease/increase during the consolidation/swelling process. Fluid elements that are adjacent to the top and bottom boundaries at time $t$ are designated as $i,m'_i$ and $i,m'_b$, respectively.
Fig. 2.7  Geometry for CST1:  (a) initial configuration, and (b) after application of vertical stress increment (Fox 2007a).
Top and bottom boundaries of the compressible layer can be specified as drained or undrained and, if drained, are assigned individual constant total head values, \( h_t \) and \( h_b \), taken with respect to the datum. Concentration boundary conditions for the top and bottom boundaries can be specified as constant concentration (Type I), constant gradient (Type II), or constant flux (Type III) (Fox 2007b). Fig. 2.7 describes Type I conditions in which the top and bottom boundaries are maintained at constant concentrations \( c_t \) and \( c_b \). Based on the computed distribution of void ratio and fluid flows across drained boundaries at each time step using CS2 algorithm, CST1 tracks the advection of fluid elements within the column (Fox 2007a).

Solute transport occurs by advection of fluid elements, dispersion between contiguous fluid elements, and sorption onto solid elements that are also moving in response to the consolidation process. The dual-Lagrangian framework of CST1 automatically accounts for advection transport in the fluid phase and sorption transport on the solid phase (Fox 2007a). Dispersion transport is calculated between contiguous fluid elements with variable porosity and seepage velocity in the associated solid elements taken into account. Mass transport through solid particles by solid-phase diffusion is neglected.
2.3.2 Solute transport

The longitudinal dispersion mass flow rate \( J_z \) is calculated as

\[
J_z = -n_{\text{eff}} D_L \frac{\partial C}{\partial z} A
\]  

(2.26)

where \( D_L = D^* + \alpha_L v_s \) is the longitudinal hydrodynamic dispersion coefficient and \( A \) is the cross sectional area. In CST1, longitudinal dispersion is calculated between vertically contiguous fluid elements using an equivalent series value for \( D_L \) based on current values of soil porosity and seepage velocity in the appropriate solid elements,

\[
D_{L,s,m} = \sum_{j=1}^{R} \frac{z_{f,m+1}^j - z_{f,m}^j}{N_{L,j,m}^t} \quad m = m_h, m_h +1, ..., m_t -1
\]  

(2.27)

where \( n_j^i \) is porosity of solid element \( j \), \( z_{f,m} \) is node elevation of fluid element \( m \), and the value of \( N_{L,j,m}^t \) depends on the relative positions of fluid zone \( i,m \) and the associated solid elements (Fox 2007a). Fluid zone \( i,m \) is defined as the area between fluid node \( i,m \) and fluid node \( i,m+1 \). For each fluid element, Eq. 2.27 performs a summation over all solid elements. The transverse dispersion mass flow rate \( J_x \), the spreading of solute in directions normal to the direction of advection, is considered in CST1 with similar calculation procedures as the longitudinal dispersion mass flow rate. Details are provided by Fox (2007a).
2.3.3 Mass balance, sorption/desorption, and decay reaction

The updated solute mass in the \( i,m \) fluid element at time \( t + \Delta t \) is calculated from inter-element mass flow rates as

\[
C_{f,i,m}^{t+\Delta t} = C_{f,i,m}^t + \left( J_{x,i-1,m}^t - J_{x,i,m}^t + J_{z,i,m-1}^t - J_{z,i,m}^t \right) \Delta t \quad i = 1, 2, \ldots, R_i
\]

\[ m = m_i^b + 1, \; m_i^b + 1, \ldots, m_i^b - 1 \] (2.28)

where \( C_{f,i,m} \) is dissolved solute mass in the \( i,m \) fluid element, \( J_{x,i,m} \) and \( J_{z,i,m} \) are the transverse and longitudinal dispersion mass flow rate, respectively, between fluid element nodes \( i,m \) and \( i,m+1 \). CST1 accounts for sorption/desorption reactions by allowing for equilibrium mass transfer between fluid and solid elements. Fluid element \( i,m \) exchanges solute mass with any solid element \( i,j \) if the node of the solid element lies within the boundaries of the fluid element. The solute mass sorbed onto solids associated with the \( i,m \) fluid element is

\[
C_{s,i,m}^{t+\Delta t} = \Delta x \sum_{j=1}^{R_j} S_{i,j}^t \rho_{d,j}^{t+\Delta t} L_{s,j}^{t+\Delta t} \quad i = 1, 2, \ldots, R_i
\]

\[ m = m_i^{b+\Delta t}, \; m_i^{b+\Delta t} + 1, \ldots, m_i^{b+\Delta t} \] (2.29)

where \( C_{s,i,m} \) is sorbed solute mass associated with the \( i,m \) fluid element, \( \Delta x \) is element width, \( S_{i,j}^t \) is the sorbed solute mass per mass of solid phase, \( \rho_{d,j}^{t+\Delta t} \) is the dry density, \( g \) is the acceleration of gravity, and \( L_{s,j} \) is the height of the \( j^{th} \) solid element. Solid elements that contribute to the summation satisfy \( (z_{s,j}^{t+\Delta t} > z_{fb,m}^{t+\Delta t}) \) and \( (z_{s,j}^{t+\Delta t} \leq z_{ft,m}^{t+\Delta t}) \), where \( z_{s,j}^{t+\Delta t} \) (\( = z_{fb,m+1}^{t+\Delta t} \)) is the elevation of the
top of fluid element $m$, and $z_{f_{i-1},m}$ ($= z_{f_i,m-1}$) is the elevation of the bottom of fluid element $m$. Solute masses in fluid and solid elements may decay over time increment $\Delta t$ according to separate first-order reactions, giving a total updated solute mass associated with the $i,m$ fluid element equal to

$$C_{f,i,m}^{t+\Delta t} = C_{f,i,m}^{t+\Delta t} (1 - \lambda_c \Delta t) + C_{s,i,m}^{t+\Delta t} (1 - \lambda_s \Delta t) \quad i = 1, 2, \ldots, R_i$$

$$m = m_h^{t+\Delta t}, \quad m_b^{t+\Delta t} + 1, \ldots, m_i^{t+\Delta t}$$ (2.30)

where $\lambda_c$ and $\lambda_s$ are lumped first-order decay constants for dissolved and sorbed solute masses, respectively. A new fluid element concentration is then calculated assuming linear equilibrium sorption between fluid and solid phases:

$$c_{i,m}^{t+\Delta t} = \frac{C_{i,m}^{t+\Delta t}}{V_{i,m}^{t+\Delta t} + \Delta t \sum_{j=1}^{R_i} K_{d,i,j} L_{i,j}^{t+\Delta t}} \quad z_{s,j}^{t+\Delta t} > z_{f_{i-1},m}^{t+\Delta t} \quad \text{and} \quad z_{s,j}^{t+\Delta t} \leq z_{f_i,m}^{t+\Delta t}$$

$$i = 1, 2, \ldots, R_i \quad \text{and} \quad m = m_h^{t+\Delta t}, \quad m_b^{t+\Delta t} + 1, \ldots, m_i^{t+\Delta t}$$ (2.31)

where $c_{i,m}$ is dissolved solute concentration the $i,m$ fluid element, $V_{f,m}$ is volume of fluid in $m$ fluid element which is invariant (Fox 2007a), and $K_{d,i,j}$ is the equilibrium distribution coefficient (sorbed concentration/aqueous concentration) for solid element $i,j$. $K_d$ is treated as a spatially-varying parameter to allow for a non-uniform distribution of soil sorption capacity, such as due to changing organic content. Possible variation of $K_d$ with changing porosity during consolidation is neglected. Finally, sorbed concentrations on solid elements associated with the $i,m$ fluid element are updated as
The accuracy of the above procedure for sorption/desorption is sensitive to the relative numerical resolution of fluid and solid elements. Some simplicity is achieved when an odd integer number of fluid elements is initially specified for each solid element. Setting \( R_{mo} = 3R_j \) is satisfactory for most sorption problems and, as such, a simulation begins with three fluid elements inside each solid element (i.e., \( L_{fo} = L_{so}/3 \)). If very large strains are expected, \( R_{mo} = 5R_j \) is specified.

### 2.3.4 Time incremental criteria

CST1 uses explicit time integration with a variable time increment \( \Delta t \). At each time step, the time increment is taken as the minimum of five values:

\[
\Delta t = \min \left\{ \frac{\alpha \gamma_a a_{v,j}^t \left( L_{s,j}^t \right)^2}{k_j^t (1 + e_j^t)}, \frac{0.01 L_a (e_{o,j}^t - e_{f,j}^t)}{(1 + e_{o,j}^t)(v_{f,j}^{t+\Delta t} - v_{f,j}^t)}, \frac{(\Delta x)^2}{8 D_{f,m}^t}, \frac{\left( L_{f,m}^t \right)^2}{8 D_{xs,m}^t}, \frac{0.01 C_{f,i,m}^t}{J_{x,i-1,m}^t + J_{x,i,m}^t + J_{z,i,m-1}^t - J_{z,i,m}^t} \right\}
\]  

\[(2.33)\]

where \( \alpha = 0.4 \), \( a_{v,j}^t \) is the coefficient of compressibility calculated at \( e_j^t \) from Fig. 2.5(a), and \( e_{f,j}^t \) is the final void ratio for solid element \( j \). Values of \( e_{f,j}^t \) are calculated from the final vertical effective stress increment assuming no unload/reload and may be approximate if unload/reload occurs. The first two terms in Eq. 2.33 are needed for numerical stability of the consolidation algorithm and accurate time
integration of discharge velocity near drainage boundaries during the early stages of a simulation (Fox and Berles 1997). The third and fourth terms provide numerical stability for the transverse and longitudinal dispersion algorithms and are based on a similar expression used by Zhu and Fox (2000). The fifth term is needed for accurate time integration of dispersion transport. CST1 also decreases the time increment as needed to properly follow the time-loading sequence $\Delta q'$ for the layer. Using these criteria, CST1 performs a search over all fluid and solid elements at each time step to find the smallest value of $\Delta t$, which is then used to advance the solution forward in time for all elements.

2.3.5 Model verification and conclusion

Verification checks of CST1 showed excellent agreement with analytical solutions for solute transport in rigid porous media (Fox 2007b). Simulations were performed for advection, diffusion, dispersion, linear equilibrium sorption, first-order decay, first-order source decay, various Peclet number, 1D and 2D transport problems, and different transport boundary conditions. Verification checks were also performed for 1D solute transport in a consolidating layer, and settlement and solute breakthrough curves are in excellent agreement with corresponding results from a large strain finite element model based on material coordinates (Fig. 2.8). The strain-invariant coefficient of consolidation $c_F^{e'}\left(=\frac{1+e_o}{1+e} c_r\right)$ was held constant for these simulations. The data from Lewis and Smith was unpublished but obtained through personal communication (Fox 2007b). Simulations using CST1 illustrate that consolidation-induced advection
can lead to significantly higher effluent concentrations than diffusion alone. The simulations also indicate that consolidation can have a lasting effect on solute migration because transient advective flows change the distribution of solute mass within a given system which then becomes the initial condition for subsequent transport processes.
Fig. 2.8 Numerical solutions for consolidation-induced VOC transport through a single composite liner system: (a) settlement, and (b) breakthrough curves (Fox 2007b).
2.4 Experimental Work

2.4.1 Centrifuge tests

A few researchers have conducted experiments to investigate consolidation-induced solute transport. Potter et al. (1994) presented the first analysis of this effect and conducted bench-top centrifuge tests to simulate the transport of contaminants through a consolidating waste deposit. The waste layer was modeled using speswhite kaolin clay contaminated with sodium chloride and was underlain by a drainage layer of silica flour. The numerical solution for effluent concentration was in good agreement with measurements, whereas solutions for pore pressure within the clay layer were significantly in error. Considering that large strains (over 50%) were achieved in the centrifuge test, this latter disparity was attributed to the small strain assumption of the numerical model. Using large diameter centrifuge tests, Potter et al. (1997) again modeled the consolidation of a contaminated kaolin clay layer and, in this case, included the application of a sand cap as shown in Fig. 2.9(a). Fig. 2.9(b) presents measured and predicted pore water pressures in the clay layer. The discrepancy between measured and predicted pore water pressures is caused by different coordinate systems. The pore pressure probe was fixed in space (15.2 m of prototype height in Fig. 2.9a), but the numerical coordinate remains at the same position within the clay during consolidation (Lagrangian coordinate, Section 2.2.2).

To see the effect of consolidation caused by centrifugation on chloride migration, concentrations of chloride were measured in the clay layer and underlying sand layer (Fig. 2.9a). Fig. 2.10(a) and (b) present the measured and predicted concentrations in the clay
layer as a function of prototype time. The numerical model predicted faster chloride migration in the clay layer. However, as shown in Fig. 2.10(c) and (d), the predicted migration of chloride in underlying sand layer was slower than measured migration. They concluded that contaminant migration was affected, at least in part, by consolidation of the clay because both measured and simulated concentrations in Fig. 2.10(a) at early time showed similar trend of measured and simulated pore pressures (Fig. 2.9b) caused by the consolidation in the clay layer.
Fig. 2.9  (a) Geometry of centrifuge tests and (b) Predicted and measured total pore water pressures (Potter et al. 1997)
Fig. 2.10  Predicted and measured concentrations at discrete points throughout the clay and underlying sand (Potter et al. 1997)
Moo-Young et al. (2001) conducted large diameter centrifuge tests to investigate consolidation-induced transport of a radiolabeled inorganic contaminant ($^{63}$Ni) and Rhodamine dye from a sediment layer into an overlying capping layer. The sediment and cap were both silty sands and exhibited low compressibility. For these tests, only a small fraction (0.50%) of the radiolabeled contaminant was lost from the sediments due to consolidation, and 0.48% of the radiolabeled contaminant was sorbed into capping material ($K_d = 339 \text{ mL/g}$). Fig. 2.11(a) shows Rhodamine dye concentration versus prototype time for the overlying water samples during the centrifuge test. Rhodamine dye is non-reactive, so this data illustrates that pore water moves from the sediment layer through the capping layer, and into the overlying water. In addition, as shown in Fig. 2.11(b), the cap decreases in water content from 38% to an average of 26% and the sediment decreases in water content from 41% to an average of 23%. Based on the centrifuge test results, they concluded that advection and dispersion were the dominant transport processes.

Using a similar method and the same centrifuge equipment, Moo-Young et al. (2003) investigated consolidation-induced transport of Rhodamine dye in high plasticity dredged clay after placement of a sand cap. Again, measurements of increasing dye concentration with time in the overlying water reservoir and final profiles of dye concentration over depth provided evidence of solute transport. As shown in Fig. 2.12, settlement measurements were in good agreement with numerical simulations from a large strain consolidation model (PSDDF) which is based on finite strain consolidation
theory described by Gibson et al. (1967). Simulations of consolidation-induced solute transport were not conducted for comparison with the measured concentration data.
Fig. 2.11  Centrifuge test results; (a) dye concentration in overlying water, and (b) water content profile for the sediment and cap (Moo-Young et al. 2001)
Fig. 2.12  Settlement comparison of numerical model (PSDDF) to centrifuge tests (Moo-Young et al. 2003)
2.4.2 Modified consolidation tests

Alshawabkeh et al. (2004) performed two replicate consolidation tests (labeled $R$ and $L$) on composite kaolinite specimens consisting of an upper layer contaminated with sodium bromide and a lower layer contaminated with sodium chloride. Fig. 2.13 shows a schematic diagram of the consolidation apparatus. Each specimen was single-drained at the top boundary and placed under a constant load of 25 kPa. The test results are in good agreement, with both specimens reaching a final strain of 8.6%. Fig. 2.14(a) shows bromide concentration in the surrounding water vs. dimensionless time factor ($T_r$) for each test. Measured settlements and bromide concentrations in a water reservoir surrounding the consolidation cell show similar trends. In addition, both rate of the consolidation settlement and bromide flux show similar behavior (Fig. 2.14b). Bromide concentration shows a high rate of change during the early stages of consolidation ($T_r < 0.5$). These data indicate that consolidation accelerated the outflow rate of bromide from the specimens. As with the Moo-Young et al. research, numerical modeling of consolidation-induced solute transport was not conducted for this study.
Fig. 2.13  Schematic diagram of the consolidation apparatus including the initial bromide distribution in the specimen. Dimensions are in mm (Alshawabkeh et al. 2004).
Fig. 2.14  Consolidation settlement and bromide concentration in the surrounding water bath vs. dimensionless time factor (Alshawabkeh et al. 2004)
2.4.3 Conclusion

The above studies have provided valuable insight into the effects of consolidation-induced solute transport. More definitive data is however needed with regard to control of concentration boundary conditions, reactive contaminant species, and different loading schedules (including diffusion-only tests) to clearly identify the contribution of consolidation to the transport process. More extensive experimental data is also needed for rigorous validation of computational models.

2.5 Effect of Clay Consolidation on Solute Transport Parameters

Accurate prediction of solute transport through the deforming porous media requires a reliable estimation of the key parameters and their response to spatially and temporally varying void ratio and effective stress caused by consolidation. Relatively little is known about the effects of changing porosity on solute transport parameters. One application that requires such data is the numerical modeling of consolidation-induced solute transport in which large strains are taken into account, such as CST1 (Fox 2007a). Several studies have been conducted on the relationship between diffusion and dispersion transport parameters and media porosity.

2.5.1 Effective diffusion and hydrodynamic dispersion coefficients

Manheim (1970) correlated the results from 22 chloride diffusion tests conducted on six sediments and showed that the effective diffusion coefficient ($D^*$) decreased with decreasing porosity. Diffusion rates through the sediments ranged from 5 to 50% of the
corresponding free solution diffusion rates. Based on this data, Lerman (1978) proposed a nonlinear (power) function relationship between \( D' \) and porosity. Myrand et al. (1992) found that a simpler linear relationship between \( D' \) and porosity was satisfactory for diffusion of volatile organic compounds through clayey soils.

Mazzieri et al. (2002) presented an investigation of dispersion transport of MgCl\(_2\) in kaolinite that included batch tests and dispersion column tests conducted at two levels of effective stress. Specimens for Test n.1 and Test n.2 were consolidation under a total stress of 50 kPa and 415 kPa, respectively. The column tests indicated that the hydrodynamic dispersion coefficient (\( D_h \)) decreased as the effective stress increased (\( D_h \) of Mg\(^{2+}\) and Cl\(^-\) = 6.11 and 5.10 \( \times \) 10\(^{-10} \) m\(^2\)/s at 50 kPa, and \( D_h \) = 1.93 and 2.53 \( \times \) 10\(^{-10} \) m\(^2\)/s at 415 kPa). Values of \( D_h \) for both nonreactive (Cl\(^-\)) and reactive (Mg\(^{2+}\)) species were in the range of effective diffusion coefficients for compacted clays (Shackelford and Daniel 1991b) and thus it was concluded that mechanical dispersion effects were negligible in these tests.

Lo et al. (2003) performed bench-scale centrifuge column tests to investigate the migration of a cadmium solution through bentonite-amended sand. The specimen for soil column test was consolidated under a total stress of 68.9 kPa. Final effective stress distribution including seepage force was 68.9 to 31.9 kPa at the top and the bottom of the specimen, respectively. For the centrifuge column test, the effective stress distribution including seepage force was 0 to 43.9 kPa. Hydrodynamic dispersion coefficients were found to be 0.25 cm\(^2\)/s for the soil column test and 0.35 cm\(^2\)/s for the centrifuge column test. Based on the experimental results in which \( D_h \) decreased with increasing 

60
effective stress, they concluded that stress state may need to be considered in the description of transport mechanisms for heavy metals in soils.

2.5.2 Sorption isotherm

Research on the relationship between sorption and media porosity (or solids content) has also been conducted using both batch tests and soil column tests. The evaluation of sorption isotherms from different test conditions must be conducted carefully because isotherms are empirical relationships that have no intrinsic thermodynamic or mechanistic meaning and are thus highly dependent on the specific test conditions. In general, the influence of solids-to-solution ratio will be minor when available surface sites are in excess (Limousin et al. 2007). As the solids content increases, the amount of surface sites may at one point become limited and, if not explicitly taken into account, this will produce a shift in the resulting isotherm (McKinley and Jenne 1991; Burgisser et al. 1993). As such, batch tests have generally yielded more sorption than column tests conducted using the same materials (Mazzieri et al. 2002; Kim et al. 2003). Mazzieri et al. (2002) also found that sorption in column tests decreased slightly with increasing effective stress as shown in Fig. 2.15. This was attributed to a larger area of solid phase involved in particle-to-particle contacts at the higher stress level. Retardation factors were, however, not significantly influenced by effective stress. Mazzieri et al. (2002) also found that batch tests overestimated the sorption in column tests (Fig. 2.15). Kim et al. (2003) recommended that batch tests should be performed with a sufficiently high solids-to-solution ratio (greater than 1:10) in
order to obtain sorption isotherms that are representative of those from column tests. In addition to the effect of solids-to-solution ratio, sorption isotherms derived from batch and column tests can also change due to different modes of mixing and solute replenishment (Burgisser et al. 1993; Porro et al. 2000, Limousin et al. 2007). Thus, although more difficult to perform than batch tests, soil column tests are generally preferred for the estimation of sorption isotherms as related to subsurface transport problems because the solids-to-solution ratio and mixing process are more similar to in situ conditions (Cherry et al. 1984, Kim et al. 2003; Limousin et al. 2007).

Fig. 2.15  Comparison of linear regression sorption isotherms from column tests and batch test (Mazzieri et al. 2002)
2.5.3 Conclusion

Published results on relationships between media porosity and transport parameters are generally consistent. It is also clear that no comprehensive study has been conducted that involves several types of tests, including consolidation tests, on a single material. In addition, some questions remain on the proper interpretation method for dispersion column tests (Parlange et al. 1992; Barry and Anderson 1996; Shackelford and Redmond 1996).

2.6 Summary

Solute transport in rigid porous media has been studied extensively for several decades. In some cases, however, such as slurry waste ponds, tailings dams, and thick landfill liners, significant volumetric strains may occur during the transport process. Coupled large strain consolidation and solute transport models have been shown to predict earlier breakthrough times for contaminants in some cases as compared to conventional rigid-media transport analysis. Experimental works such as centrifuge and consolidation tests suggest that transient advective transport caused by consolidation governs the movement of contaminants, but the data are quite limited and have not been rigorously compared to computational results.

The CS2 piecewise-linear model for the prediction of large strain consolidation has proven to be both reliable and robust. A new approach for the simulation of coupled nonlinear large strain consolidation and solute transport is based on the piecewise-linear method and is coded in the numerical model CST1. In this research, experimental data
on coupled large strain consolidation and solute transport will be compared with computation results. However, CST1 cannot accommodate changing effective diffusion coefficient during consolidation and nonlinear nonequilibrium sorption. CST2 is an improved computational model that represents the next level of sophistication beyond the model CST1. A complete presentation of the formulation and capabilities of CST2 is provided in next chapter.
CHAPTER 3
CST2 NUMERICAL MODEL

3.1 Introduction

A new approach for the simulation of coupled nonlinear large strain consolidation and solute transport is based on the piecewise-linear method and is coded in the numerical model CST2 (Consolidation and Solute Transport 2), which is based on the code CST1 for coupled large strain consolidation and solute transport (Fox 2007a). The consolidation algorithm in CST1 is one-dimensional and accounts for the effects of vertical strain with associated geometric and material nonlinearities. The solute transport algorithm in CST1 is two-dimensional and accounts for advection, dispersion, first-order decay reactions, and linear equilibrium sorption. CST2 has all the capabilities of CST1 and, in addition, can accommodate variation of effective diffusion coefficient during consolidation, nonlinear nonequilibrium sorption, and reservoir
boundary condition. For simplicity, this research focuses on the vertical (i.e., longitudinal) transport capabilities of CST2. The development of CST2 is first presented, followed by verification checks using analytical and numerical solutions for solute transport through rigid porous media. A parametric study is then presented and conclusions are reached with regard to the importance of variable effective diffusion coefficient and nonlinear nonequilibrium sorption for consolidation-induced solute transport.

3.2 Model Development

CST2 was developed using CST1 as a point of departure and follows the same procedures with regard to constitutive relationships, initial void ratio distribution, surcharge loading, settlement, and advection of fluid elements. Detailed descriptions of these aspects are presented by Fox and Berles (1997) and Fox (2007a, 2007b). The following sections focus on the additional capabilities of the CST2 model.

3.2.1 Geometry

A saturated homogeneous soil layer of initial height $H_o$ is treated as an idealized two-phase material in which the solid particles and pore fluid are incompressible. The term “homogeneous” refers to the compressibility and hydraulic conductivity constitutive relationships of the layer and not the initial distribution of void ratio within the layer. Although soil consolidation and solute transport will generally occur in three dimensions, the following development is restricted to that of one-
dimensional consolidation and transport model. The initial geometry of the soil layer, prior to the application of a vertical stress increment at time $t = 0$, is shown in Fig. 3.1(a). The solid phase is represented as a column of $R_j$ elements. Vertical coordinate $z$ is defined as positive upward (against gravity) from a fixed datum at the base of the layer. Solid element coordinate $j$ is defined similarly. Each $j^{th}$ solid element has initial height $L_{so}$, unit cross sectional area (horizontal plane), a central node located at initial elevation $z_{so,j}$, and initial void ratio $e_{o,j}$. The distribution of void ratio is assumed to be uniform within each solid element and varies vertically depending on the initial vertical effective stress at the top of the layer $q_a$, the compressibility and self weight of the soil, and any vertical seepage forces due to an external hydraulic gradient acting across the column (Fox 2007a).

The fluid in the soil layer is also represented as a column of elements, with $R_{mo}$ fluid elements initially in the column. Fluid elements are defined by vertical element coordinate $m$. Each $m^{th}$ fluid element has initial height $L_{fo}$, unit cross sectional area, and a central node located at initial elevation $z_{fo,m}$. For cases without sorption/desorption, the initial positions of fluid and solid elements are coincident (i.e., $R_{mo} = R_j$ and $L_{fo} = L_{so}$). This is the configuration shown in Fig. 3.1(a). For cases involving sorption/desorption, higher numerical resolution is needed for the fluid phase (i.e., $R_{mo} > R_j$ and $L_{fo} < L_{so}$) and the fluid in each solid element is divided into an odd integer number (typically 3) of smaller fluid elements. The fluid in each fluid element
\( m \) has initial dissolved solute concentration \( c_{o,m} \) [mass solute/volume fluid] and initial dissolved solute mass \( C_{fo} = c_{o,m}V_{fo,m}, \) where \( V_{fo,m} = L_{fo}e_{o,j} / (1 + e_{o,j}) \) is initial volume of fluid in the element and \( e_{o,j} \) is the void ratio of the solid element at the same elevation. The initial concentration of sorbed solute mass for each solid element is assumed to be in equilibrium with the fluid concentration.

Top and bottom boundaries of the compressible layer can be specified as drained or undrained and, if drained, are assigned individual constant total head values, \( h_t \) and \( h_b, \) taken with respect to the datum. Concentration boundary conditions for the top and bottom boundaries can be specified as prescribed concentration (Type I), prescribed gradient (Type II), or prescribed mass flux (Type III). Fig. 3.1 shows Type I conditions in which the top and bottom boundaries are maintained at constant concentrations \( c_t \) and \( c_b. \) CST2 can also accommodate a reservoir boundary condition (Shackelford and Daniel 1991b).

A time dependent effective stress increment \( \Delta q' \) is applied to the layer beginning at time \( t = 0 \) and moves with the top boundary thereafter. Excess pore pressures created as a result of the stress increment cause fluid flow from the interior of the soil layer to all drainage boundaries. Soil deformation occurs in response to the net fluid outflow from each solid element. Solute transport occurs by advection and dispersion in the fluid phase and sorption onto moving solid elements. Fig. 3.1(b) shows the configuration of the system at some later time \( t. \)
Fig. 3.1. Geometry for CST2: (a) initial configuration ($t < 0$), and (b) after application of vertical stress increment ($t > 0$).
Fluid and solid elements are laterally separated for clarity but, similar to Fig 3.1(a), occupy the same physical space. Fluid elements become vertically disconnected from their original solid elements and move in response to the seepage velocity field. At time $t$, the height of the layer is $H'$, the height and void ratio of the $j^{th}$ solid element are $L_{s,j}'$ and $e_j'$, and the height of the $m^{th}$ fluid element is $L_{f,m}'$. Solid elements and fluid elements have node elevations $z_{s,j}'$ and $z_{f,m}'$, respectively, that are updated at each time step. Nodes translate vertically and remain at the center of their respective elements throughout the consolidation process. Fluid elements have concentration $c_{m}'$ and dissolved solute mass $C_{f,m}'$. Fluid elements always contain their original fluid volume $V_{f,m}$ unless they are adjacent to a drainage boundary. Thus, for problems involving consolidation (as opposed to swelling), the height of fluid elements will increase as the porosity of the associated soil elements decreases. Fluid elements move through, and possibly out of, the consolidating layer in response to excess pore pressures and any external hydraulic gradient (if $h_i \neq h_b$). Thus, unlike the number of solid elements which is always constant, the number of fluid elements may decrease/increase during the consolidation/swelling process. Fluid elements that are adjacent to the top and bottom boundaries at time $t$ are designated as $m_i'$ and $m_b'$, respectively. Based on the computed distribution of void ratio and fluid flows across drained boundaries at each time step, CST2 uses the same Lagrangian method as CST1 to track the advection of fluid elements within the column (Fox 2007a).
3.2.2 Solute transport

The dual-Lagrangian framework of CST2 automatically accounts for advection transport in the fluid phase and sorption transport on the solid phase. Longitudinal dispersion between vertically contiguous fluid elements is calculated using an equivalent series hydrodynamic dispersion coefficient $D_{ls}$ based on current values of soil porosity and seepage velocity in the associated solid elements. In the calculation of $D_{ls}$, CST1 assumes that the effective diffusion coefficient $D'$ is constant. In CST2, $D'$ varies with solid element porosity as (Lerman 1978),

$$D'_{j} = (n'_{j})^M D_o$$

(3.1)

where $n'_{j}$ is the total porosity of the $j^\text{th}$ solid element at time $t$, $M$ is a constant, and $D_o$ is the free-solution diffusion coefficient.

Figure 3.2 illustrates the calculation of $D_{ls}$ with a variable effective diffusion coefficient for three solid elements ($j-1$, $j$, and $j+1$) and three fluid elements ($m-1$, $m$, and $m+1$). The longitudinal dispersion mass flow rate $J'_{z,m}$ between fluid element $m$ and $m+1$ is

$$J'_{z,m} = -D'_{ls,m} i'_{cz,m}$$

(3.2)

where the vertical solute concentration gradient $i'_{cz,m}$ is

$$i'_{cz,m} = \frac{c'_{m+1} - c'_{m}}{z'_{f,m+1} - z'_{f,m}}$$

(3.3)

and the equivalent series hydrodynamic dispersion coefficient between nodes $m$ and $m+1$ is
Fig. 3.2. Fluid flow between contiguous solid elements, and dispersion mass flux between contiguous fluid elements.
Details for the calculation of \( N_{L,j,m}^t \) are provided by Fox (2007a). For the example shown in Fig. 3.2,

\[
\sum_{j=1}^{R_i} N_{L,j,m}^t \frac{N_{L,j,m}^t}{n_j^t} = \frac{z_{j,m+1}^t - z_{j,b,j+1}^t}{n_j^{t+1}D_{j}^{t+1} + \alpha_L v_{RF,j}^f} + \frac{z_{st,j}^t - z_{j,m}^t}{n_j^tD_j^{t+1} + \alpha_L v_{RF,j}^f}
\]  

(3.5)

where \( z_{st,j}^t \) is the elevation of the top of solid element \( j \), \( z_{sh,j+1}^t (= z_{st,j}^t) \) is the elevation of the bottom of solid element \( j+1 \), \( \alpha_L \) is the longitudinal dispersivity, and \( v_{RF,j}^f \) is the relative discharge velocity (positive upward) between solid elements \( j \) and \( j+1 \). Eq. 3.5 indicates that CST2 accounts for diffusion as well as mechanical dispersion transport effects. If mechanical dispersion is neglected (\( \alpha_L = 0 \)),

\[
D_{Ls,m}^t = \frac{z_{j,m+1}^t - z_{j,m}^t}{n_j^{t+1}D_{j}^{t+1} + \alpha_L v_{RF,j}^f}
\]

(3.6)

which indicates that \( D_{Ls} \) is simply the weighted average of two diffusion coefficients that act in series over two separate sections of the fluid column between nodes \( m \) and \( m+1 \).

3.2.3 Mass balance, sorption-desorption, and solute reactions

CST2 accounts for sorption/desorption reactions by permitting solute mass transfer between fluid and solid elements (Fig. 3.2). The general case corresponds to
the following nonlinear nonequilibrium (i.e., kinetic) sorption model (Travis and Etnier 1981):

\[
\frac{\partial s}{\partial t} = \lambda \left( K_p c^F - s \right) \tag{2.3}
\]

As in CST1, mass transfer occurs between fluid and solid elements when the fluid element encloses the solid element node. To ensure good accuracy, a larger number of fluid elements are typically specified (e.g., \( R_{mo} = 3R_j \)) such that only one fluid element exchanges solute mass with one solid element at any given time step.

The updated solute mass \( C^{t+\Delta t}_{j,m} \) in each fluid element at time \( t + \Delta t \) is calculated from inter-element mass flow rates and sorption/desorption mass transfer as

\[
C^{t+\Delta t}_{j,m} = C^t_{j,m} + \left( J^t_{z,m-1} - J^t_{z,m} \right) \Delta t = \Delta s \rho_{d,j}^{t+\Delta t} I^{t+\Delta t}_{s,j}
\]

where \( \Delta s = \lambda \left( K_p^{t} \left( c^F_{m} \right)^{t} - s^t_{j} \right) \Delta t \), \( s^t_{j} \) is sorbed solute mass per mass of solid phase, 
\( \rho_{d,j}^{t+\Delta t} = \rho_w G_s / (1 + e_{j}^{t+\Delta t}) \) = updated dry density, \( \rho_w \) is density of water (constant). In (3.7), the node of solid element \( j \) is within the boundaries of fluid element \( m \) (i.e., \( z_{s,j}^{t+\Delta t} > z_{jh,m}^{t+\Delta t} \) and \( z_{s,j}^{t+\Delta t} \leq z_{jf,m}^{t+\Delta t} \)). Like CST1, CST2 uses explicit time integration with a variable time increment \( \Delta t \) that is based on several conditions related to numerical stability and accuracy (Fox 2007a). Once the value of \( C^{t+\Delta t}_{j,m} \) is known, the updated fluid element concentration is

\[
c^{t+\Delta t}_{m} = \frac{C^{t+\Delta t}_{j,m}}{V^{t+\Delta t}_{f,m}}
\]

and the sorbed solute mass concentration for solid element \( j \) is
Conceptually, equilibrium sorption can be achieved using the above kinetic model with $\lambda \to \infty$. Use of a large $\lambda$ value, however, requires a very small time increment to avoid nonphysical oscillations in solute concentrations (Zhou and Selim 2001). To increase computational efficiency, CST2 uses a direct method to calculate sorption/desorption for nonlinear equilibrium conditions. The updated solute mass in the $m^{th}$ fluid element is

$$
C_{f,m}^{t+\Delta t} = C_{f,m}^{t} + \left(J_{z,m-1}^{t} - J_{z,m}^{t}\right)\Delta t
$$

(3.10)

and the solute mass sorbed onto solid element $j$ (node within fluid element $m$) is

$$
C_{s,m}^{t+\Delta t} = s'\rho_{d,j}^{t+\Delta t} L_{s,j}^{t+\Delta t}
$$

(3.11)

The total solute mass $C_{m}^{t+\Delta t}$ associated with fluid element $m$ is then equal to

$$
C_{m}^{t+\Delta t} = C_{f,m}^{t+\Delta t} + C_{s,m}^{t+\Delta t}
$$

(3.12)

This total mass is partitioned between fluid element $m$ and solid element $j$ according to $s = K_{p}c^{F}$. The new fluid element concentration $c_{m}^{t+\Delta t}$ is calculated from

$$
C_{m}^{t+\Delta t} = c_{m}^{t+\Delta t}L_{f,m}^{t+\Delta t} + K_{p,j}\left(c_{m}^{t+\Delta t}\right)^{F}\rho_{d,j}^{t+\Delta t} L_{s,j}^{t+\Delta t}
$$

(3.13)

and the equilibrium sorbed concentration is

$$
S_{j}^{t+\Delta t} = K_{p,j}\left(c_{m}^{t+\Delta t}\right)^{F}
$$

(3.14)

If $F = 1$, the foregoing method reduces to a linear equilibrium model where

$$
S_{j}^{t+\Delta t} = K_{d,j}c_{m}^{t+\Delta t}
$$

(3.15)
and $K_{d,j}$ is the distribution coefficient for solid element $j$. Eq. 3.13 with linear equilibrium sorption reduces to Eq. 2.31 for the one-dimensional case.

### 3.3 Model Verification

Fox (2007b) presented a series of verification checks for CST1 that demonstrate the accuracy of the model for solute transport in rigid and deformable porous media, including prescribed solute concentration (Type I), prescribed solute gradient (Type II) and prescribed solute mass flux (Type III) boundary conditions. CST2 has the same capabilities and accuracy as CST1 and, in addition, can accommodate variable effective diffusion coefficient, nonlinear nonequilibrium sorption, and reservoir boundary condition. Verification checks for these aspects are presented for rigid porous media in the following sections.

#### 3.3.1 Variable effective diffusion coefficient

The capability of CST2 to simulate solute transport for conditions of a spatially varying effective diffusion coefficient was evaluated for two cases of layered rigid porous media. The geometry is shown in Fig. 3.3. An initially uncontaminated porous column having total height $H = 0.5$ m is composed of two layers with heights $H_1 = 0.05$ m and $H_2 = 0.45$ m and constant effective diffusion coefficients $D_1^*$ and $D_2^*$. Both layers have porosity $n = 0.4$. Boundary heads of $h_b = 1.5$ m and $h_t = 1.0$ m give a steady upward seepage velocity of $v_s = 1 \times 10^{-7}$ m/s. At time $t = 0$, a non-reactive solute is introduced at the bottom boundary using a flux-controlled boundary
condition (Type III) with constant $c_o$. The outflow condition at the top boundary is zero concentration gradient (Type II). Mechanical dispersion is neglected ($\alpha_L = 0$).

Variable effective diffusion coefficient

Fig. 3.3  Geometry for solute transport through rigid layered porous media.
Solute transport through the column was simulated using CST2 with $R_j = 200$ solid elements and $R_{mo} = 200$ initial fluid elements. Two cases were considered: (1) $D_1^* = 1 \times 10^{-9} \text{ m}^2/\text{s}$ and $D_2^* = 4 \times 10^{-10} \text{ m}^2/\text{s}$, and (2) $D_1^* = 4 \times 10^{-10} \text{ m}^2/\text{s}$ and $D_2^* = 1 \times 10^{-9} \text{ m}^2/\text{s}$. A small modification to CST2 was required to accommodate different $D^*$ values for the same porosity. Profiles of relative concentration $c/c_o$ are shown in Fig. 3.4 for simulations terminated at $t = 5 \text{ d}$ and $10 \text{ d}$. Analytical solutions obtained using the equations of Leij and van Genuchten (1995) are also shown for comparison. The Leij and van Genuchten solutions are approximate for this problem because the first layer is finite ($H_1 = 0.05 \text{ m}$) and the second layer is semi-infinite ($H_2 = \infty$). However, these solutions provide a very good approximation because the top boundary solute concentration is negligible at $t = 10 \text{ d}$. Fig. 3.4 shows that the CST2 numerical simulations are in excellent agreement with the corresponding analytical solutions.
Fig. 3.4  Solute concentration profiles for solute transport through rigid layered porous media with a spatially varying effective diffusion coefficient.
3.3.2 Nonlinear equilibrium sorption

An additional simulation was performed for a homogeneous column (no layers) with nonlinear equilibrium sorption. The initially uncontaminated column has \( H = 0.5 \, \text{m} \), \( G_s = 2.7 \), \( n = 0.4 \), \( v_s = 5 \times 10^{-8} \, \text{m/s} \), \( D^* = 5 \times 10^{-10} \, \text{m}^2/\text{s} \), and \( \alpha_L = 0 \).

A reactive solute \( (K_p = 5 \, \text{mL/g}, \ F = 0.7) \) is introduced at the bottom boundary with constant concentration \( c_b = c_o \) (Type I). The top boundary (outflow) condition is zero concentration gradient (Type II). The column was modeled using CST2 with \( R_j = 200 \) and \( R_{mo} = 600 \). Fig. 3.5 shows the simulated breakthrough curve and fluid concentration profiles at \( t = 250 \, \text{d} \) and \( 500 \, \text{d} \). Numerical solutions were also obtained using the computer software program HYDRUS-1D v3.0 (Simunek et al. 2005) with 600 elements. Excellent agreement is observed.
Fig. 3.5  Solute transport through rigid porous media with nonlinear equilibrium sorption: (a) breakthrough curve; (b) fluid concentration profiles.
### 3.3.3 Linear nonequilibrium sorption

Oddson et al. (1970) presented analytical solutions for advective transport ($\alpha_L = 0$ and $D^* = 0$) of a reactive solute with linear nonequilibrium sorption that can be reproduced in CST2. Simulations were performed for $H = 0.5$ m, $G_s = 2.7$, $n = 0.4$, $v_s = 4 \times 10^{-7}$ m/s, $K_d = 10$ mL/g, $R_j = 200$, $R_{mo} = 600$, and values of $\lambda$ ranging from $1 \times 10^{-8}$/s to $1 \times 10^{-6}$/s. Both boundaries were modeled using prescribed concentration (Type I) conditions. Solute concentration at the bottom (inflow) boundary was increased to $c_o$ for $t = 0$ to 1 d and then reduced to zero thereafter. The top (outflow) boundary was maintained at zero concentration. Fig. 3.6(a) shows relationships for solute breakthrough at elevation $z = 0.05$ m along with corresponding analytical solutions. Smaller values of $\lambda$ correspond to slower rates of solute sorption/desorption and hence higher values of relative fluid concentration. Profiles of dissolved and sorbed solute concentrations, shown in Figs. 3.6(b) and 3.6(c), are presented at four times for $\lambda = 1 \times 10^{-7}$/s and at $t = 3$ d for five $\lambda$ values. Analytical and numerical solutions are again in excellent agreement.
Fig. 3.6  Solute transport through rigid porous media with linear nonequilibrium sorption: (a) breakthrough curves; (b) fluid concentration profiles; and (c) sorbed concentration profiles.
Fig. 3.6 continued

![Graph showing relative sorbed concentration vs. elevation for different time periods and decay coefficients.](image)

- CST2
- \( \lambda = 5 \times 10^{-7} \text{s}^{-1} \)
- \( \lambda = 5 \times 10^{-8} \text{s}^{-1} \)
- \( \lambda = 1 \times 10^{-6} \text{s}^{-1} \)
- \( \lambda = 1 \times 10^{-7} \text{s}^{-1} \)
- \( \lambda = 1 \times 10^{-6} \text{s}^{-1} \)
3.3.4 Reservoir boundary

A final verification check for CST2 was performed for a reservoir boundary condition. The geometry is shown in Fig 3.7. A well-mixed aqueous reservoir containing a nonreactive solute with initial concentration $c_o$ overlies an initially uncontaminated soil specimen. For conditions of diffusion only ($v_s = 0$), Shackelford and Daniel (1991b) presented a closed form solution for reservoir concentration $c_{res}'$ at any time $t$ after the start of diffusion. A simulation was performed using CST2 for $H = 0.1$ m, $H_r = 0.1$ m, $n = 0.4$, $D' = 5 \times 10^{-10}$ m$^2$/s, $R_j = 200$, and $R_{mo} = 200$. The top boundary condition is prescribed concentration (Type I) with $c_i' = c_{res}'$ and $c_{res}'$ updated at each time step based on the loss of solute mass into the soil. The bottom boundary condition is zero flux. Fig. 3.8 shows excellent agreement between analytical and numerical solutions for the change of reservoir concentration with time.
Fig. 3.7  Geometry for diffusion transport through rigid porous media with reservoir boundary condition.
Fig. 3.8 Reservoir concentration versus time for diffusion transport with reservoir boundary condition.

3.4 Parametric Study

A parametric study was conducted to investigate the significance of variable effective diffusion coefficient and nonlinear nonequilibrium sorption on consolidation-induced solute transport. CST2 was used to simulate solute transport for a hypothetical single-increment consolidation test of a layered clay slurry specimen. The geometry is shown in Fig. 3.9. An uncontaminated clay slurry layer with a thickness of 10 mm
overlies a contaminated layer with a thickness of 70 mm, giving total initial height $H_o = 80$ mm. The contaminated layer contains a reactive solute with a uniform initial dissolved concentration $c_o = 400$ mg/L and a corresponding equilibrium sorbed concentration for the soil solids. The initial vertical effective stress $q_o$ at the top boundary is 2 kPa.

Fig. 3.9  Geometry for single-increment consolidation test of layered clay slurry specimen: (a) initial configuration; (b) after application of stress increment.
An effective stress increment $\Delta q = 200$ kPa is applied at $t = 0$ and held constant for two days (48 h). All transport processes also begin at $t = 0$. Pore fluid is not removed from the consolidation cell and thus settlement creates an aqueous reservoir above the soil specimen with depth $H'_i = H_o - H'$ and total head $h_i = H_o$. The top boundary was modeled using the reservoir boundary condition and the bottom boundary is assumed to be zero-flux for both pore fluid and solute mass. As such, all advective flow is upward and results in the transport of solute mass through the uncontaminated layer and into the reservoir.

Material properties for both layers were taken from measurements reported by Fox (1996) for a clay slurry ($G_s = 2.78$, $LL = 112$, $PL = 56$). Constitutive relationships for compressibility and hydraulic conductivity are

$$e = e_o - C_c \log \left( \frac{\sigma'_v}{\sigma'_{w0}} \right)$$  \hspace{1cm} (3.16)

$$k = k_o \left(10^{\frac{e - e_o}{C_c}} \right)$$  \hspace{1cm} (3.17)

where $\sigma'_v$ is vertical effective stress, $k$ is vertical hydraulic conductivity, $e_o = 4.34$, $\sigma '_ o = 0.946$ kPa, $C_c = 1.02$, $k_o = 2.04 \times 10^{-8}$ m/s, and $C_k = 1.3$. The initial void ratio distribution is nearly uniform and ranges from 4.01 at the top of the specimen to 3.95 at the bottom (variation due to self weight). The free solution diffusion coefficient for the solute is $D_o = 1 \times 10^{-9}$ m$^2$/s and mechanical dispersion is neglected ($\alpha_L = 0$). All CST2 simulations were performed with $R_j = 200$ and $R_{mo} = 600$. 

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3.4.1 Variable effective diffusion coefficient

The first set of simulations was performed to investigate the effect of variation of $D^*$ during consolidation for conditions of linear equilibrium sorption ($K_p = 5 \text{ mL/g, } F = 1$). Soil solids in the contaminated layer are initially in equilibrium with $c_o$ and have a uniform initial sorbed concentration $s_o = 2000 \text{ mg/kg}$. Considering the data of Lerman (1978) in which $M$ ranges from 1.2 to 2.8 for various sediments, four simulations were conducted using CST2 for $M = 0, 1, 2,$ and 3. The variation of $D^*$ with porosity is shown in Fig. 3.10 for each case. The average initial porosity for the specimen is 0.80 and the average final value is 0.66.

Specimen settlement and reservoir concentrations are presented as a function of time in Fig. 3.11(a). The applied effective stress increment (200 kPa) produces a final settlement of 32.4 mm and a final average strain of 40.5%. Elapsed times corresponding to average degree of consolidation $U_{avg} = 30\%, 60\%, \text{ and 90\% are 1.74, 7.02, and 18.0 h, respectively.}$ Solute concentrations do not affect the consolidation process and, hence, the settlement curve in Fig. 3.11(a) applies to all simulations performed for the parametric study. Reservoir concentration increases with time for each simulation, with larger $c_{res}$ values observed for larger $D^*$ values (smaller $M$). Rates of increase in reservoir concentration are high during the early stages of consolidation and then decrease subsequently. After consolidation is completed, reservoir concentration continues to increase, albeit at a slower rate, due to upward diffusion of solute.
Fig. 3.10  Variation of effective diffusion coefficient with porosity.

Fig. 3.11(a) also shows three additional reservoir concentration curves for advection only (no diffusion) and for diffusion only (no consolidation) with $M = 2$. The diffusion simulations correspond to the initial geometry and the final geometry of the specimen, and thus should bracket the true “diffusion only” $c_{res}$ values for the deforming specimen. These curves illustrate that both advection and diffusion acting in isolation produce relatively little transport to the reservoir. However, when acting together, these processes produce much higher $c_{res}$ values. Similar to the findings of Fox (2007b),

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consolidation has a lasting effect on solute migration because transient advective flows change the distribution of solute mass within the specimen (i.e., move it closer to the top), which then becomes the initial condition for subsequent diffusion processes.

Corresponding profiles of solute concentration are shown in Fig. 3.11(b) for $U_{\text{avg}} = 30\%$, $U_{\text{avg}} = 60\%$, and $t = 48$ h (final condition). The height $H$ of the specimen is also indicated for each set of profiles. As time and settlement increase, the concentration profile changes from a relatively sharp front to a more gradual transition through the specimen. Higher values of $D^*$ accelerate solute transport and tend to further smooth the concentration profile. At 48 h, fluid concentration in the uncontaminated layer reaches significant levels, depending on the value of $D^*$. Fig. 11 indicates that, for this example, varying effective diffusion coefficient has an important effect on consolidation-induced solute transport.
Fig. 3.11 Consolidation-induced solute transport for variable effective diffusion coefficient: (a) settlement and reservoir concentrations; and (b) fluid concentration profiles.
3.4.2 Nonlinear equilibrium sorption

The effect of sorption isotherm nonlinearity was investigated by performing one simulation for a linear isotherm \( K_d = 5 \text{ mL/g, } F = 1 \) and three simulations for nonlinear isotherms, all shown in Fig. 3.12. The nonlinear isotherms were chosen such that linear regression over the concentration range \( c = 0 \) to 400 mg/L produces the same relationship as the linear isotherm and, as such, the results can be directly compared. The initial sorbed concentrations \( s_o = K_p c_o^F \) are different in each case; thus, the contaminated layers have different initial sorbed and total solute masses. The value of \( D^* \) was constant \( (1 \times 10^{-9} \text{ m}^2/\text{s}) \) for each simulation.

Fig. 3.13(a) shows reservoir concentration as a function of time for each simulation. Although the curves appear to be essentially parallel, they do converge slightly with time. The linear isotherm produces the highest \( c_{res} \) values because the uncontaminated layer has the lowest sorptive capacity for \( c < 285 \text{ mg/L} \) (Fig. 3.12), which is true for each of the four simulations. Conversely, the isotherms become more nonlinear as \( F \) decreases, which leads to greater sorption in the uncontaminated layer and slower solute breakthrough. The effect of isotherm nonlinearity on final fluid concentration profiles (Fig. 3.13b) is small. Corresponding sorbed concentration profiles (Fig. 3.13c) indicate a more important effect for the initially uncontaminated layer, with \( s/s_o \) values at the top ranging from 0.45 to 0.62. Fig. 3.13 suggests that, for this example, isotherm nonlinearity has a relatively unimportant effect on consolidation-induced solute transport.
Fig. 3.12  Linear and nonlinear sorption isotherms.
Fig. 3.13  Consolidation-induced solute transport for nonlinear equilibrium sorption: (a) settlement and reservoir concentrations; (b) fluid concentration profiles; and (c) sorbed concentration profiles.
3.4.3 Linear nonequilibrium sorption

A final set of simulations was performed to investigate the importance of nonequilibrium sorption effects during consolidation. For simplicity, the isotherm is taken as linear ($K_d = 5 \text{ mL/g}$, $F = 1$) and $D^*$ is constant ($1 \times 10^{-9} \text{ m}^2/\text{s}$). Soil solids in the contaminated layer have a uniform initial sorbed concentration $s_o = 2000 \text{ mg/kg}$. Reservoir concentrations are shown in Fig. 3.14(a) for six values of kinetic sorption parameter $\lambda$ (Eq 2.3). The value $\lambda = 0$ indicates no sorption/desorption process can
occur in either layer (i.e., initial sorbed concentrations remain constant) and the value \( \lambda = \infty \) corresponds to equilibrium sorption in both layers. For this example, the curve for \( \lambda = 1 \times 10^{-3}/s \) essentially matches the equilibrium response and produces the lowest reservoir concentrations. As \( \lambda \) decreases, reservoir concentrations increase due to less solute sorption in the uncontaminated layer. Interestingly, reservoir concentrations approach the final value much faster for low values of \( \lambda \). Fig. 3.14(a) also shows that the difference between equilibrium and nonequilibrium curves at low \( \lambda \) is greatest during the early stages of consolidation when the advection rate is the highest and the time available for solute equilibration is the least. As required, these curves converge for large times as shown in Fig 3.14(b). Fluid and sorbed concentration profiles, shown in Figs. 3.14(c) and 14(d) for \( U_{avg} = 30\% \) and \( t = 48 \) h (final condition), are consistent with the trends of Fig. 3.14(a). Faster rates of sorption produce lower fluid concentrations and higher sorbed concentrations in the uncontaminated layer.
Fig. 3.14 Consolidation-induced solute transport for linear nonequilibrium sorption: (a) settlement and reservoir concentrations; (b) reservoir concentrations for large times (c) fluid concentration profiles; and (d) sorbed concentration profiles.
Fig. 3.14 continued

(c) Relative Fluid Concentration, \( c/c_0 \)
(d) Relative Sorbed Concentration, \( s/s_0 \)
The effect of rate of consolidation on the importance of kinetic sorption is illustrated in Fig. 3.15. Two sets of simulations are presented for linear equilibrium ($K_d = 5 \text{ mL/g}, \lambda = \infty$) and linear nonequilibrium ($K_d = 5 \text{ mL/g}, \lambda = 1 \times 10^{-5}/\text{s}$) sorption. For each set, three simulations were performed using $2k_o$, $k_o$, and $0.5k_o$ in the hydraulic conductivity constitutive relationship (Eq 3.17). When hydraulic conductivity values are twice as fast ($2k_o$), settlement occurs more quickly, and when hydraulic conductivity values are twice as slow ($0.5k_o$), settlement occurs more slowly than for the original relationship ($k_o$). As the rate of consolidation increases, differences in reservoir concentrations for equilibrium and nonequilibrium sorption conditions become more pronounced. Interestingly, the nonequilibrium curve for fastest consolidation shows a reservoir concentration that reaches a peak at $t = 10.5 \text{ h}$ and then decreases with time. Initially, advective transport causes a rapid rise in reservoir concentration with little sorption in the uncontaminated layer. As advection slows down, a reverse transport process occurs in which solute mass diffuses back into the clay specimen and is sorbed into the uncontaminated layer, thus reducing the reservoir concentration. Figs. 3.14 and 15 indicate that, for this example, nonequilibrium sorption can have a strong effect on consolidation-induced solute transport and that this effect becomes more important as the rate of consolidation increases.
Fig. 3.15. Effect of rate of consolidation on reservoir concentrations for consolidation-induced solute transport with linear equilibrium and nonequilibrium sorption.
3.5 Summary

CST2 is a computational model for coupled large strain consolidation and solute transport in saturated porous media that represents the next level of sophistication beyond the model CST1 (Fox 2007a, 2007b). The consolidation algorithm is one-dimensional and accounts for vertical strain, soil self-weight, general constitutive relations, relative velocity of fluid and solid phases, changing hydraulic conductivity and compressibility during consolidation, time-dependent loading, unload/reload effects, and an external hydraulic gradient acting across the layer. Constitutive relationships for the soil are defined using discrete data points and can take nearly any desired form. The solute transport algorithm of CST2 is also one-dimensional and accounts for advection, longitudinal dispersion, changing effective diffusion coefficient during consolidation, first-order decay reactions, and nonlinear nonequilibrium sorption. Solute transport is consistent with temporal and spatial variations of porosity and seepage velocity in the consolidating layer. The key to the transport model is the definition of two Lagrangian fields of elements that follow the motions of fluid and solid phases separately. This reduces numerical dispersion and simplifies transport calculations to that of dispersion mass flow between contiguous fluid elements. CST2 provides the following quantities as a function of time: 1) settlement of the consolidating layer, 2) solute concentration in the pore water effluent, and 3) total solute mass outflow from the layer. CST2 also provides the following quantities as a function of time and position within the consolidating layer: 1) void ratio, 2) pore pressure, 3) dissolved solute concentration, and 4) sorbed solute concentration.
Verification checks of CST2 show excellent agreement with analytical and numerical solutions for solute transport in rigid porous media. A parametric study conducted using CST2 illustrates that, for the test cases considered, variation of effective diffusion coefficient during consolidation has an important effect on solute transport, whereas nonlinearity of the sorption isotherm has a less important effect. Additional simulations show that nonequilibrium (i.e., kinetic) sorption can have a strong effect on consolidation-induced solute transport and that this effect becomes more important as the rate of consolidation increases. The simulations also corroborate previous findings of Fox (2007b) that consolidation can have a lasting effect on solute migration because transient advective flows change the distribution of solute mass within a given system which then becomes the initial condition for subsequent transport processes.
The experimental program was conducted to: 1) investigate the effect of clay consolidation on solute transport parameters, 2) investigate the significance of consolidation-induced solute transport for well-controlled conditions, and 3) validate CST2 simulations of consolidation-induced solute transport. This chapter described batch tests, diffusion column tests, dispersion column tests, consolidation tests, and solute transport tests. The materials and procedures for these tests are described in this chapter.
4.1 Materials

All tests were performed on specimens of kaolinite clay. The kaolinite was purchased from the Unimin Corporation in powdered form and has a specific gravity of solids \( G_s = 2.61 \), liquid limit \( LL = 47.6 \), and plasticity index \( PI = 21.8 \). The material is classified according to the Unified Soil Classification System as CL, Lean Clay. Transport tests were conducted using dilute solutions of potassium bromide (KBr). An inorganic solute consisting of potassium bromide (KBr) was selected to evaluate solute transport. A standard solute solution was prepared by dissolving KBr salt in deionized water. \( \text{Br}^- \) is a non-reactive tracer and \( \text{K}^+ \) experiences sorption/desorption due to the cation exchange capacity of the kaolinite. The cation exchange capacity was determined by a method in which kaolinite is expanded with 0.5 M NaCl\(_2\), and then washed repeatedly with a saturating solution of 0.5 M CaCl\(_2\). The kaolinite (saturated with Ca\(^{2+}\)) is rinsed with 95% ethanol, and exposed to a 0.5 M MgCl\(_2\) solution to determine the release of Ca\(^{2+}\) which is the CEC of the kaolinite. The measured CEC of kaolinite was 6.5 meq/100g. Additional Atterberg limit tests conducted with KBr solution (860 mg/L Br\(^-\), 421 mg/L K\(^+\)) as pore fluid yielded \( LL = 46.8 \) and \( PI = 20.3 \), which are slightly lower than the values obtained using deionized water.
4.2 Batch Tests

Four batch tests were conducted at a nominal pH of 7.5 ± 0.2 using 75 mL glass tubes with a 1:10 solids-to-solution ratio (5 g kaolinite, 50 g KBr solution) and initial concentrations of KBr solution ranging from 134 to 646 mg/L. The tubes were continuously stirred for two days using a reciprocating shaker table and solution concentrations were measured beginning at 3 min of elapsed time using ion-selective electrodes manufactured by Cole-Parmer (Models 27504-26 and 27502-05), with a reproducibility of ±2%. Sorbed concentrations were calculated from the difference between the initial and final dissolved solute masses.

4.3 Soil Column Tests

4.3.1 Diffusion column tests

Eight diffusion column tests were performed to determine the effective diffusion coefficient $D^*$ at different values of porosity. Table 4.1 provides a summary of these tests. Specimens of uncontaminated kaolinite were prepared with initial water contents ranging from approximately 0.9 LL to 2.2 LL, which correspond to initial void ratios $e_v$ ranging from 1.15 to 2.73. The specimens were placed in glass columns (dia. = 48 mm), manufactured by Kontes (Model 420830), to a height of 150 mm as shown in Fig. 4.1. Specimens C1 to C6 were placed by spooning with care taken not to entrain air into the material during this process.
<table>
<thead>
<tr>
<th>Test</th>
<th>$e_o$</th>
<th>$e_f$</th>
<th>$n$</th>
<th>Initial concentration $c_o$ (mg/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Br$^-$</td>
</tr>
<tr>
<td>C1</td>
<td>2.73</td>
<td>2.70</td>
<td>0.73</td>
<td>820</td>
</tr>
<tr>
<td>C2</td>
<td>2.48</td>
<td>2.49</td>
<td>0.71</td>
<td>861</td>
</tr>
<tr>
<td>C3</td>
<td>2.24</td>
<td>2.26</td>
<td>0.69</td>
<td>846</td>
</tr>
<tr>
<td>C4</td>
<td>1.86</td>
<td>1.90</td>
<td>0.66</td>
<td>821</td>
</tr>
<tr>
<td>C5</td>
<td>1.49</td>
<td>1.54</td>
<td>0.61</td>
<td>849</td>
</tr>
<tr>
<td>C6</td>
<td>1.49</td>
<td>1.56</td>
<td>0.61</td>
<td>854</td>
</tr>
<tr>
<td>C7</td>
<td>1.20</td>
<td>1.16</td>
<td>0.54</td>
<td>839</td>
</tr>
<tr>
<td>C8</td>
<td>1.15</td>
<td>1.10</td>
<td>0.52</td>
<td>877</td>
</tr>
</tbody>
</table>

Table 4.1. Summary of conditions for diffusion column tests.

Specimens C7 and C8 were prepared to higher water contents, placed in the columns, and then consolidated under a surcharge pressure of 80 kPa (top-drained). The specimens were consolidated in small layers so that side friction was not a problem. Each layer was allowed to be consolidated for three days, so the specimens were prepared after two weeks. The surcharge was removed and the C7 and C8 specimens were permitted to swell to equilibrium. A deionized water reservoir was then added to each column to a depth of 70 mm and the specimens were sealed and permitted to sit undisturbed for a minimum of two weeks to achieve equilibrium with regard to volume change. The deionized water reservoir was then removed and an equal volume of KBr solution with an initial concentration $c_o$ was added to each column. The columns then
sat for an additional 100 days. During this time, the reservoirs were gently stirred each day to eliminate fluid concentration gradients. The concentration of Br\(^-\) and K\(^+\) in each reservoir was periodically measured by electrode. After the testing period was completed, final water contents were measured, which yielded the values of final void ratio \(e_f\) provided in Table 4.1. Initial and final void ratios are nearly equivalent, indicating that no significant volume change occurred during these tests. The porosity \(n\) reported for each test corresponds to the final void ratio.
Fig. 4.1. Diffusion column test apparatus.
4.3.2 Dispersion column tests

Five dispersion column tests were performed to obtain the hydrodynamic dispersion coefficient \( D_h \), longitudinal dispersivity \( \alpha_h \), and sorption isotherm at different values of porosity. The first two parameters are defined by Eq. 2.2. Table 4.2 provides a summary of test conditions and Fig. 4.2 shows a diagram of the test apparatus. Specimens were placed in a glass column (dia. = 25 mm) to a height \( H = 50 \) mm using the same procedures as for the diffusion tests (specimens D4 and D5 were consolidated similarly to specimens C7 and C8). A syringe flow pump, manufactured by Harvard Apparatus (Model 44), was connected to the base of the column to provide steady upward flow of KBr solution through the specimens. Inflow solutions were prepared to a target concentration of 818 mg/L Br\(^-\) and 400 mg/L K\(^+\). Actual inflow concentrations \( c_o \) are listed in Table 4.2. Pore water pressures were measured at the base of each specimen using a pressure transducer (Validyne Model DP15). A flow adapter (Kontes Model 420876-1620) with small diameter (1.6 mm) tubing was inserted into each column to more quickly remove the effluent water for sampling. Effluent samples were taken at time increments corresponding to a flow of 0.25 pore volume and concentrations of Br\(^-\) and K\(^+\) were measured using electrodes. Final water contents were measured at the conclusion of each test and yielded the final void ratios provided in Table 4.2. Final void ratios are in close agreement with the initial values, indicating that no significant volume change occurred as a result of advection during these tests.
Table 4.2. Summary of conditions for dispersion column tests.

<table>
<thead>
<tr>
<th>Test</th>
<th>$e_o$</th>
<th>$e_f$</th>
<th>$n$</th>
<th>$i$</th>
<th>$k$ ($\times 10^{10}$ m/s)</th>
<th>$v_s$ ($\times 10^8$ m/s)</th>
<th>Initial concentration $c_o$ (mg/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>D1</td>
<td>2.24</td>
<td>2.36</td>
<td>0.70</td>
<td>3.38</td>
<td>252</td>
<td>12.17</td>
<td>860</td>
</tr>
<tr>
<td>D2</td>
<td>1.86</td>
<td>1.83</td>
<td>0.65</td>
<td>22.23</td>
<td>44.0</td>
<td>15.05</td>
<td>872</td>
</tr>
<tr>
<td>D3</td>
<td>1.49</td>
<td>1.62</td>
<td>0.62</td>
<td>16.18</td>
<td>30.7</td>
<td>8.01</td>
<td>837</td>
</tr>
<tr>
<td>D4</td>
<td>1.20</td>
<td>1.14</td>
<td>0.53</td>
<td>122.7</td>
<td>5.78</td>
<td>13.38</td>
<td>876</td>
</tr>
<tr>
<td>D5</td>
<td>1.15</td>
<td>1.03</td>
<td>0.51</td>
<td>67.63</td>
<td>3.52</td>
<td>4.67</td>
<td>848</td>
</tr>
</tbody>
</table>
Fig. 4.2. Dispersion column test apparatus.
4.4 Consolidation Tests

Two incremental loading consolidation tests were performed to determine compressibility and hydraulic conductivity constitutive relationships and any variation of these relationships with pore fluid chemistry. Using the same procedures and apparatus as the consolidation-induced transport tests (described subsequently), these tests were conducted on an uncontaminated kaolinite specimen and a uniformly contaminated kaolinite specimen prepared using KBr solution (398 mg/L K⁺, 813 mg/L Br⁻). Hydraulic conductivity measurements were obtained in between load increments using a syringe flow pump connected to the base of the cell. These tests began once consolidation was completed, as determined from settlement and pore pressure data. Upward flow was used to decrease effective stress within the specimens and thus avoid additional consolidation. Settlement measurements confirmed that void ratio remained constant during permeation. The hydraulic conductivity tests lasted approximately 24 h each and had a maximum hydraulic gradient of 18. Permeants used for hydraulic conductivity testing of the uncontaminated and uniformly contaminated kaolinite specimens were deionized water and KBr solution, respectively.
4.5 Solute Transport Tests

4.5.1 Specimen preparation

The solute transport experiments consisted of one diffusion transport test (J6) and six consolidation-induced transport tests (J1-J5, J7). Each of these tests was conducted on a composite kaolinite specimen consisting of an upper “uncontaminated” kaolinite slurry layer and a lower “contaminated” kaolinite slurry layer. The target water content for each layer was 95.2 % (= 2 LL). The uncontaminated kaolinite slurry was prepared using deionized water and cured on a shaker table for a minimum of one week. The contaminated kaolinite slurry was prepared using the KBr solution (1635 mg/L Br⁻, 800 mg/L K⁺) and was also cured on a shaker table for one week to ensure equilibrium sorption prior to testing. Daily measurements of pore fluid concentration indicated no change after the first day.

The experimental apparatus is shown in Fig. 4.3. Contaminated and uncontaminated slurry layers were placed in a rigid wall cell (dia. = 102 mm) by a combination of spooning and pouring. Care was taken to remove entrapped air from the test cell apparatus and to entrain as little air as possible into the slurry during this process. Filter paper was placed adjacent to porous discs at the top and bottom of the specimen and in between the slurry layers to provide separation. The inner walls of the cell were coated with thin layers of lubricant oil in an effort to reduce side friction. Table 4.3 presents the initial layer heights, initial void ratios \( e_o \), initial pore fluid concentrations for the lower layer \( c_o \), number of loading steps, and top boundary conditions for the solute transport tests. The bottom boundary condition for each test was zero flux with
regard to both pore fluid and solute mass. Initial potassium concentrations in the contaminated layers are below the standard solution concentration (800 mg/L) due to potassium sorption onto the solid phase. Each test began immediately after the composite specimen was prepared to minimize diffusion transport into the upper uncontaminated layer prior to testing.
Fig. 4.3 Composite kaolinite slurry specimen and consolidation test apparatus.
<table>
<thead>
<tr>
<th>Test</th>
<th>Uncontaminated Layer (top)</th>
<th>Contaminated Layer (bottom)</th>
<th>Loading step</th>
<th>Concentration Boundary (c&lt;sub&gt;i&lt;/sub&gt;)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Height (mm)</td>
<td>e&lt;sub&gt;o&lt;/sub&gt;</td>
<td>Height (mm)</td>
<td>e&lt;sub&gt;o&lt;/sub&gt;</td>
</tr>
<tr>
<td>J1</td>
<td>21.1</td>
<td>2.51</td>
<td>50.6</td>
<td>2.46</td>
</tr>
<tr>
<td>J2</td>
<td>19.4</td>
<td>2.48</td>
<td>50.4</td>
<td>2.45</td>
</tr>
<tr>
<td>J3</td>
<td>18.2</td>
<td>2.52</td>
<td>50.4</td>
<td>2.51</td>
</tr>
<tr>
<td>J4</td>
<td>52.1</td>
<td>2.54</td>
<td>19.0</td>
<td>2.52</td>
</tr>
<tr>
<td>J5</td>
<td>56.9</td>
<td>2.56</td>
<td>15.3</td>
<td>2.46</td>
</tr>
<tr>
<td>J6</td>
<td>52.2</td>
<td>2.55</td>
<td>21.0</td>
<td>2.59</td>
</tr>
<tr>
<td>J7</td>
<td>17.5</td>
<td>2.51</td>
<td>51.1</td>
<td>2.50</td>
</tr>
</tbody>
</table>

<sup>a</sup> including unload/reload

Table 4.3 Summary of solute transport tests
4.5.2 Diffusion transport test

One diffusion transport test (J6) was conducted using the consolidation test apparatus (Fig. 4.3) with no load applied to the specimen and with no water reservoir above the specimen. The top and bottom boundaries of the specimen thus corresponded to zero flux with regard to both fluid and solute mass. The cell was covered to prevent evaporation and allowed to sit undisturbed for 18 days. After the diffusion period was completed, the test specimen was carefully sampled over its depth using a spoon (due to the high water content) to obtain profiles of final water content and dissolved and sorbed concentrations. Samples were placed in 30 mL tubes and centrifuged for 10 min. The supernatant was then manually extracted using a pipette and the Br\(^{-}\) and K\(^{+}\) concentrations were measured by electrode. To measure sorbed concentrations of K\(^{+}\), pore water that remained in the solid phase after centrifugation was removed using a filter press. Two grams of each dry filter cake was then placed in a centrifuge tube along with 20 mL of 0.7 M nitric acid. The centrifuge tubes were placed on a shaker table for two days and then centrifuged. K\(^{+}\) concentrations in the nitric acid solution were measured by Inductively Coupled Plasma–Atomic Emission Spectroscopy (Australia Vista Ax ICP-AES) and the sorbed mass of K\(^{+}\) was calculated. Since there was no settlement, pore pressure, or fluid and solute outflows, the final concentration profiles were the only measurements obtained for the J6 diffusion test.

4.5.3 Consolidation-induced transport tests

Six one-dimensional, incremental-loading consolidation tests (J1 – J5, J7) were conducted on similar composite (i.e., layered) kaolinite specimens to directly measure
consolidation-induced solute transport. Each composite specimen was loaded in the consolidation cell (Fig. 4.3) to a maximum vertical stress of 78.4 kPa with single drainage at the top boundary and pore pressure measurements taken at the base. Thus, advection occurred upward from the contaminated layer and through the uncontaminated layer. The tests varied with regard to initial thickness of the slurry layers, loading schedule, and top boundary concentration conditions (Table 4.3).

Tests J1 – J3 were designed to investigate the effect of top boundary concentration condition. These specimens had a thick contaminated (lower) layer and were subjected to identical loading schedules (3.1 - 5.6 - 10.4 - 20.1 - 39.5 - 78.4 kPa). Each load increment remained on the specimens for 3 days, with primary consolidation generally finished in approximately 2 days. Therefore, the total testing time for J1 – J3 was 18 days each. The bottom boundary condition was zero concentration gradient (Type II). The top boundary for J1 was also maintained as zero concentration gradient (Type II) by continuously removing all pore water effluent using a peristaltic pump manufactured by MasterFlex (Model 7554-90). The inflow line to the pump (Tygon LFL, MasterFlex Model 06429-13) was inserted through a snug-fitting hole in the load plate such that it collected pore fluid at the top boundary as soon as it was expelled into the porous disk (Fig. 4.3). Effluent solute concentrations were measured periodically by electrode. For J2, the outflow solution was not removed (except for sampling) and thus accumulated above the specimen to form a reservoir. Reservoir concentration changed with time due to solute mass outflow. Concentration gradients in the reservoir were eliminated by continuous recirculation of the reservoir solution using a peristaltic pump. For J3, a second peristaltic pump was used to provide clean (deionized) water
continuously to the top boundary of the specimen, but at a slower rate than the withdrawal pump. Thus, a reservoir was not permitted to accumulate and the top boundary was maintained at zero concentration \( (c = 0, \text{ Type I}) \) throughout the test. Effluent concentrations were not measured for J3 due to the dilution effect.

Tests J4 – J6 were designed to investigate the effect of loading schedule. These specimens had thinner contaminated (lower) layers than J1 – J3 and were subjected to the same zero-gradient top boundary concentration condition (Type II) as J1 by continuous removal of the effluent solution. The loading schedule for J4 was the same as for J1 – J3. The loading schedule for J5 consisted of two increments (3.1, 78.4 kPa) at 3 days each and thus J5 reached the final stress much faster than J4. J6 is the diffusion test described previously and thus had no applied load over an 18-d test period.

Test J7 was designed to be a more complicated consolidation-induced solute transport test and included an unload/reload stage along with changing concentration conditions at the top boundary. No reservoir was permitted to accumulate at anytime. The loading schedule consisted of 12 load increments (3.1 - 5.6 - 10.4 - 20.1 - 39.5 - 10.4 - 3.1 - 10.1 - 39.5 - 78.4 - 20.1 - 3.1 kPa) at 3 days each. For the first loading sequence (3.1 - 5.6 - 10.4 - 20.1 - 39.5 kPa), the top boundary condition was maintained at zero concentration gradient (Type II), similar to J1. The specimen was then unloaded (10.4 - 3.1 kPa) with zero concentration (i.e., clean deionized water, Type I) at the top boundary, similar to J3. As such, any soil swelling during this unloading sequence would draw clean water into the specimen. Reloading (10.1 - 39.5 - 78.4) and final unloading (20.1 - 3.1 kPa) were again conducted under conditions of zero concentration gradient and zero
concentration, respectively. As with J3, solute mass outflows during the unloading stages were not measured due to the dilution effect.

After the last load increment was completed for each consolidation-induced transport test, the specimen was unloaded completely, extruded from the consolidation cell, and sliced into horizontal disks to obtain profiles of final water content and dissolved and sorbed concentrations (using the same method as described for J6). Average final void ratios for the six tests ranged from 1.18 to 1.30.
Results of the experimental and numerical investigations are presented in this chapter. The effect of clay consolidation on solute transport parameters are first discussed based on the results of batch, soil column, and solute transport tests. This section includes an investigation of the preferred interpretation method for dispersion column tests as some questions remain unanswered (Parlange et al. 1992, Barry and Anderson 1996, Shackelford and Redmond 1996). Consolidation and solute transport parameters are determined for input data to the numerical simulations. Measured and simulated consolidation results are then presented and include settlement, excess pore pressure, and final void ratio profiles. The remainder of the chapter presents the extensive results and discussions of the experimental and numerical investigations of consolidation-induced solute transport.
5.1 Effect of Clay Consolidation on Solute Transport Parameters

5.1.1 Sorption data

Equilibrium sorption data for $\text{K}^+$ measured from the batch and solute transport tests is shown in Fig. 5.1(a). Fluid concentrations for the batch tests correspond to a low solids-to-solution ratio, whereas fluid concentrations for the solute transport tests represent pore scale (i.e., resident) values. All isotherms are nonlinear and show generally good agreement with the Freundlich equation ($s = K_p c^F$). Values of $K_p$ and $F$ from the batch tests are 31.8 mL/g and 0.564, respectively, whereas values from the consolidation tests are 19.56 mL/g and 0.608. The batch and solute transport data are in reasonable agreement and similar to the findings of Mazzieri et al. (2002) and Kim et al. (2003). The batch data indicate higher levels of sorption as shown in Fig. 5.1(a). This deviation in the data sets is consistent with the literature and represents the inherent differences in the two test methods (Limousin et al. 2007). Points corresponding to the initial concentration conditions of the slurry specimens for the solute transport tests are also shown. These data points are in good agreement with the final measured values and suggest that kaolinite porosity had little effect on sorption for the solute transport tests. Results of the kinetic batch tests, in which $s$ was determined as a function of time, are presented in Fig. 5.1(b). Although the data show some variability, equilibrium concentrations were generally achieved in approximately 30 min. The curves were fitted using a finite difference solution to the nonlinear kinetic sorption equation (Eq 2.3) with a value of $\lambda$ equal to 0.005/s.
Fig. 5.1. Measured and calculated sorption isotherm from batch and solute transport tests: (a) equilibrium sorption isotherms and (b) kinetic sorption effect for K⁺ and kaolinite.
5.1.2 Dispersion data

Few analysis methods/packages are readily available to calculate solute transport parameters from experimental breakthrough curves with isotherm nonlinearity taken into account. As the batch and solute transport tests clearly indicate nonlinear sorption for K$^+$ (Fig. 5.1a) analysis of measured breakthrough curves was conducted using the finite element model HYDRUS-1D (v3.0, Simunek et al. 2005). The required input data are $n$, $c_o$, discharge velocity ($k_i$), boundary conditions, type of sorption isotherm, and the concentration variable ($c_r$ or $c_f$). HYDRUS-1D performs a regression analysis to obtain a simulated breakthrough curve and provides values for $D_h$, $K_h$, and $F$. Fig. 5.2 presents measured and simulated breakthrough curves for dispersion column tests D1 and D3. The simulated curves for these tests represent the worst and best fits to the experimental data, respectively. Corresponding data from all dispersion tests is presented in Appendix A. Complete breakthrough of Br$^-$ occurred in 10 to 20 days, whereas breakthrough of K$^+$ was delayed due to sorption. Simulated breakthrough curves for Br$^-$ using Method II and III (Section 2.1.4) are very close to the measured data, whereas simulated curves using Method I show slightly slower solute transport in some cases. The only significant difference occurs for specimen D1. All simulated curves for K$^+$ are in close agreement with the measured data. Simulated Br$^-$ curves using Method I are closer to the measured data if HYDRUS-1D is permitted to choose its own value of effective porosity. However, the model experienced convergence problems when using this approach for the K$^+$ data. Thus, total porosity $n$ was specified for all simulations and the analyses were performed with the assumption that effective porosity
is equal to total porosity. This is consistent with experimental results for clayey soils by Rowe et al. (1988) and Kim et al. (1997) in which effective porosity was found to be essentially the same as total porosity.
Fig. 5.2  Measured and simulated breakthrough curves for dispersion column tests:  

(a) D1, and (b) D3.
Table 5.1 presents values of $D_h$, $K_p$, and $F$ for the simulated breakthrough curves using each analysis method. In general, values of $D_h$ decrease with decreasing void ratio, which is in agreement with the findings of Mazzieri et al. (2002) and Lo et al. (2003). $D_h$ values obtained using Method I are generally closer to those obtained from Method II. Method III estimates the highest values for $D_h$. Interestingly, Shackelford and Redmond (1996) found similar results in which $D_h$ values calculated using analytical solutions for a finite column (similar to Method III) were slightly larger than corresponding values obtained using the semi-infinite approximation (similar to Methods I and II). The $D_h$ values for $K^+$ are higher than those for $Br^-$ in almost all cases. This is in agreement with the data of Shackelford and Redmond (1995) in which dispersion coefficients for a reactive solute ($Na^+$) were two to three times greater than those for a non-reactive solute ($Cl^-$).
<table>
<thead>
<tr>
<th>Test</th>
<th>Method I</th>
<th>Method II</th>
<th>Method III</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Br⁻</td>
<td>K⁺</td>
<td>Br⁻</td>
</tr>
<tr>
<td>D₁</td>
<td>Dₜ</td>
<td>Dₜ</td>
<td>Kₚ</td>
</tr>
<tr>
<td></td>
<td>× 10⁻¹⁰ m²/s</td>
<td>× 10⁻¹⁰ m²/s</td>
<td>mL/g</td>
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<tr>
<td>D₁</td>
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<td>29.78</td>
<td>3.83</td>
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<td>D₂</td>
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<td>67.93</td>
<td>59.11</td>
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<td>D₃</td>
<td>5.29</td>
<td>19.95</td>
<td>13.56</td>
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<td>D₄</td>
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<td>7.52</td>
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<tr>
<td>D₅</td>
<td>3.92</td>
<td>17.29</td>
<td>10.72</td>
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</tbody>
</table>

Table 5.1. Summary of parameters for dispersion column tests
Figure 5.3 presents sorption isotherms for the dispersion column tests, as back-calculated using Methods I, II and III, along with the measured data from batch and solute transport tests previously shown in Fig. 5.1(a). Isotherms obtained using Method I show the best agreement with the measured data with regard to magnitude and nonlinearity. On the other hand, isotherms obtained using Methods II and III are generally more linear and indicate greater sorption than the batch and solute transport data, particularly at higher fluid concentration levels. Based on Fig. 5.3, dispersion transport parameters obtained using Method I were used for the remainder of this research.
Fig. 5.3  Sorption isotherms from batch, solute transport, and dispersion tests obtained using:  (a) Method I, (b) Method II, and (c) Method III.
5.1.3 Diffusion data

Data from the diffusion column tests is used to obtain values of effective diffusion coefficient $D^*$ and apparent tortuosity factor $\tau_a$. Measured reservoir concentrations of Br$^-$ and K$^+$ for diffusion column test C1 are shown in Fig. 5.4 as a function of time. Reservoir concentrations for both species decreased over the 100 d testing period at a progressively decreasing rate. Analysis of the Br$^-$ data is more straightforward than the K$^+$ data because sorption is not involved. A single value of $D^*$ was obtained from the Br$^-$ data using the analysis method of Shackelford and Daniel (1991b). The method produces a close fit to the measurements and yields $D^* = 11.39 \times 10^{-10}$ m$^2$/s.
Corresponding plots for the other seven diffusion tests show very similar trends and closeness of fit (Appendix B). Each $D^*$ value was then used to calculate the apparent tortuosity factor $\tau_a = D^* / D_o$, where $D_o = 20.8 \times 10^{-10} \text{ m}^2/\text{s}$ is the free solution diffusion coefficient for Br$^-$ (Shackelford and Daniel 1991a). The resulting values of $D^*$ and $\tau_a$ for Br$^-$ are presented in Table 5.2. In general, both values tend to decrease with decreasing void ratio.

![Diagram of measured and simulated curves](image)

Fig. 5.4 Measured and simulated curves for diffusion column test C1.
<table>
<thead>
<tr>
<th>Test</th>
<th>$D^*$ (× 10^{-10} m^2/s)</th>
<th>$\tau_a$</th>
<th>$D^*$ Method A (× 10^{-10} m^2/s)</th>
<th>$D^*$ Method B (× 10^{-10} m^2/s)</th>
<th>$D^*$ Method C (× 10^{-10} m^2/s)</th>
<th>$\tau_a$</th>
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<td>11.39</td>
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<td>10.58</td>
<td>10.96</td>
<td>9.30</td>
<td>0.47</td>
</tr>
<tr>
<td>C6</td>
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<td>0.38</td>
<td>7.45</td>
<td>8.52</td>
<td>7.72</td>
<td>0.39</td>
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<tr>
<td>C7</td>
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</table>

Table 5.2  Summary of parameters for diffusion column tests
Calculation of diffusion parameters for K\(^+\) was again complicated by the nonlinear isotherm. Three methods were used to determine \(D^*\) for each test. For the first method (Method A), \(D^*\) is calculated using the apparent tortuosity factor obtained from the Br\(^-\) data for the same test and the value of \(D_o\) for K\(^+\) (i.e., \(D^* = \tau_a D_o\), where \(D_o = 19.6 \times 10^{-10}\) m\(^2\)/s). For Method B, the K\(^+\) diffusion data was analyzed using the method of Shackelford and Daniel (1991b) and assuming linear sorption. The specified distribution coefficient \(K_d\) for these analyses (2.33 mL/g) was taken as the average secant slope from all five dispersion isotherms over the fluid concentration range 0 – 400 mg/L (Fig. 5.3(a)). For Method C, the diffusion data was fitted by trial and error using the numerical model CST2. For this work, CST2 was used to simulate diffusion with constant void ratio, zero advection, and a nonlinear equilibrium isotherm. The specified Freundlich constants for these analyses (\(K_p = 11.99\) mL/g, \(F = 0.708\)) were obtained by regression from all five dispersion test isotherms over the fluid concentration range 0 – 400 mg/L (Fig. 5.3(a)). In CST2, the reservoir concentration was assumed to be uniform (i.e., well mixed) and was updated at each time step based on loss of solute mass into the clay. The concentration at the top boundary was equal to that of the reservoir and the bottom boundary condition was modeled as zero concentration flux.

Diffusion transport parameters for K\(^+\) as determined by Methods A, B, and C are presented in Table 5.2. Method C values are considered to be most accurate because the capabilities of the CST2 model most closely fit the conditions of the diffusion tests. Apparent tortuosity factors were calculated using values of \(D^*\) obtained from Method C and \(D_o = 19.6 \times 10^{-10}\) m\(^2\)/s. Similar to the Br\(^-\) data, \(D^*\) and \(\tau_a\) tend to decrease
with decreasing void ratio. Simulated reservoir concentrations for K\(^+\) obtained using Methods B and C, shown for test C1 in Fig. 5.4, are in excellent agreement with the measured data and yield \(D^*\) values for K\(^+\) of 9.87 and \(9.20 \times 10^{-10}\) m\(^2\)/s, respectively. Similar excellent agreement was obtained using both methods for the other seven diffusion tests (Appendix B). Fig. 5.5 shows a comparison of \(D^*\) values obtained using each method and indicates that the first two methods generally produce larger values than Method C. Interestingly, \(D^*\) values obtained using Method A cross over those from Method C as \(D^*\) increases whereas values obtained using Method B display a nearly constant offset.

Figure 5.6(a) shows a plot of \(D^*\) (Method C) versus porosity for Br\(^-\) and K\(^+\). Also shown are two regression curves obtained using following nonlinear relationship (Lerman 1978),

\[
D^* = (n)^M D_o
\]  

(5.1)

for values of \(M = 1.69\) (Br\(^-\)) and 1.95 (K\(^+\)). Lerman (1978) found that \(M\) ranged from 1.2 to 2.8 for six sediments and thus the calculated \(M\) values are within the expected range. Fig. 5.6(a) shows that \(D^*\) decreases with decreasing porosity and that Br\(^-\) values are generally larger than corresponding K\(^+\) values. Values of apparent tortuosity factor, shown in Fig. 5.6(b), bring the data together slightly because \(D_o\) for Br\(^-\) is higher than for K\(^+\). A single regression curve defined by,

\[
\tau_a = (n)^M
\]  

(5.2)

where \(M = 1.815\), provides a satisfactory fit to this data.
Fig. 5.5  Comparison of $D^*$ values for $K^+$ obtained using three methods.
Fig. 5.6  Variation of:  (a) effective diffusion coefficient with porosity, and
(b) apparent tortuosity factor with porosity.
5.1.4 Dispersivity

A value of longitudinal dispersivity ($\alpha_L$) was calculated for each dispersion column test and ion species using Eq. (2.2), $D_h$ (Table 5.1, Method I), $v_s$ (Table 4.2), and $D^*$. Values of $D^*$ were calculated using Eq. 5.2 and the appropriate values of $D_o$ and $n$ (Table 4.2). Fig. 5.7 shows a plot of $\alpha_L$ versus void ratio for Br$^-$ and K$^+$. Values for K$^+$ are significantly larger than those for Br$^-$, which results primarily from differences in the respective $D_h$ values. Dispersivity differences for K$^+$ and Br$^-$ may be due to other cations moving through the system (e.g. Na$^+$ release as K$^+$ is sorbed). If all cation concentrations had been measured, $\alpha_L$ of K$^+$ might have been gotten to be the same as that of Br$^-$. Both plots show no clear trend with decreasing void ratio and yield average values of $\alpha_L$ equal to 0 and 20 mm for Br$^-$ and K$^+$, respectively. The low value of $\alpha_L$ for Br$^-$ is consistent with comments of Gillham and Cherry (1982) who state that $\alpha_L$ values determined in the laboratory (usually for tracers) generally range from 0.1 to 10 mm and Fried (1972) who suggested 1 mm as an average value. This is also consistent with the results of Klotz and Moser (1974) in which grain size and uniformity coefficient were found to substantially affect dispersion in column tests. Thus, the small grain size and high uniformity coefficient for the current tests would be expected to produce a low $\alpha_L$ value for tracer transport. The different values of $\alpha_L$ determined for Br$^-$ and K$^+$ are consistent with the previous discussion of the dispersion of nonreactive and reactive solutes (Section 5.1.2).
Fig. 5.7  Variation of longitudinal dispersivity with void ratio.
5.1.5 Summary and transport parameters

Based on Figs. 5.1(b) and 5.3(a), the numerical simulations were performed with $K_p = 19.56 \text{ mg/L}$, $F = 0.608$, and $\lambda = 0.005/\text{s}$. Similar to the findings of Mazzieri et al. (2002) and Kim et al. (2003), the batch data indicate higher levels of sorption due to the significantly lower solids-to-solution ratio and more efficient mixing process for these tests. As a such, $K_p$ and $F$ values were taken from the isotherm measured directly from the solute transport tests. Seven data points corresponding to the initial concentrations of $K^+$ in the contaminated (lower) layers of the solute transport tests, shown in Fig. 5.1(a), are in good agreement with points from the final concentration profiles, which suggests that changing kaolinite porosity during consolidation had little effect on $K^+$ sorption.

The diffusion column tests yielded values of apparent tortuosity factor $\tau_a$ that decreased with decreasing porosity, as shown in Fig. 5.6(b). The data for $\text{Br}^-$ and $K^+$ are in good agreement and were fitted using a nonlinear equation (Eq 5.2) with $M = 1.815$ and $D_o = 2.08 \times 10^{-9} \text{ m}^2/\text{s}$ for $\text{Br}^-$ and $1.96 \times 10^{-9} \text{ m}^2/\text{s}$ for $K^+$ (Shackelford and Daniel 1991a). Values of $\alpha_L$ for $K^+$ were significantly larger than those for $\text{Br}^-$, which results primarily from differences in the respective $D_h$ values. As such, constant values of $\alpha_L = 0$ for $\text{Br}^-$ and $\alpha_L = 20 \text{ mm}$ for $K^+$ were used for the numerical simulations.

5.2 Consolidation Data

Consolidation behavior (i.e., settlement and pore pressures) takes on particular significance in this work because good predictions of consolidation-induced transport are
not possible if the advective flow regime is not accurately modeled. The following
sections present experimental data and numerical simulations for the consolidation
behavior of the kaolinite specimens.

5.2.1 Constitutive relationships

Compressibility relationships from the consolidation tests and consolidation-
induced transport tests are shown in Fig. 5.8(a). Essentially constant values of
compression index \( C_c = 0.65 \) and recompression index \( C_r = 0.025 \) are indicated.
Data for the uncontaminated specimen shows greater nonlinearity on the semilog plot and
slightly lower void ratios than the data for the uniformly contaminated specimen.
Compressibility curves for the consolidation-induced transport tests (J1 – J5, J7) are in
close agreement with the data for the uniformly contaminated specimen. Fig. 5.8(b)
presents hydraulic conductivity relationships for the uncontaminated and uniformly
contaminated consolidation tests and the dispersion column tests. The data are in close
agreement and yield a linear relationship on the semi-log plot with a change of hydraulic
conductivity index \( C_k = \frac{de}{d \log k} = 0.765 \). This figure also shows that pore fluid
chemistry had no effect on kaolinite hydraulic conductivity.
Fig. 5.8 Constitutive relationships for kaolinite: (a) compressibility, and (b) hydraulic conductivity.
Similar to the findings of Al-Tabbaa and Wood (1987), Nagaraj et al. (1994) and Fox (2007b), Fig. 5.8(b) indicates that hydraulic conductivity follows the same relationship for normally consolidated and overconsolidated conditions.

5.2.2 Settlement, pore pressure, and final void ratio

Consolidation data for tests J2, J5 and J7 are shown in Figs. 5.9 – 5.11. The results for J2 (Fig. 5.9) are very similar to the results for tests J1, J3 and J4 (Appendix C), which had identical loading schedules. Fig. 5.9(a) presents vertical total stress $\sigma$, and settlement $S$ as a function of time for all load increments. Settlement increased with increasing $\sigma$, to a final value of 24.5 mm, which corresponds to an average vertical strain of 35%. Excess pore pressures at the base of the J2 specimen (Fig. 5.9b) show progressively increasing maximum values with increasing load increments and indicate that consolidation was completed in each case prior to the next load application. The measured consolidation response for J5, shown in Fig. 5.10, includes a large load increment (75.3 kPa) that was applied after the initial load of 3.1 kPa. The resulting maximum measured excess pore pressure was 73.1 kPa, which is equal to 97% of the applied load. This agreement is considered excellent in the absence of backpressure. The measured consolidation response for J7 (Fig. 5.11) included two unloading stages during which excess pore pressures were negative and minor swelling occurred. The profile of final void ratio, as obtained from water contents of the slices, is nearly uniform for each test. The trend of slightly increasing void ratio with depth may result from side friction.
Fig. 5.9  Experimental data and numerical simulations for J2:  (a) settlement, (b) pore pressure, and (c) final void ratio.
All three tests show similar settlement and pore pressure responses during the first load increment (3.1 kPa) and average strains at 78.4 kPa (35%, 38% and 36%, respectively). Thus, the consolidation behavior of the consolidation specimens appears to be comparable. Settlement readings taken after primary consolidation for all tests showed insignificant secondary compression.
Fig. 5.10. Experimental data and numerical simulations for J5: (a) settlement, (b) pore pressure, and (c) final void ratio.
Numerical simulations for settlement, excess pore pressure, and final void ratio were obtained using CST2 and are also shown in Figs. 5.9 – 5.11. The simulations were conducted for single drained conditions using 200 solid elements and assuming a uniform initial void ratio for each specimen equal to the weighted average of $e_o$ values in Table 4.3. The numerical simulations are in truly excellent agreement with the experimental measurements for each test. Part of the reason for the close agreement of the settlement simulations is that measured compressibility curve for each J test (Fig. 5.8a) was used as input for CST2. As a result, the final settlement for each load increment was matched to the measured value.
Fig. 5.11 Experiment data and numerical simulations for J7: (a) settlement, (b) pore pressure, and (c) final void ratio.
This procedure was used to eliminate unnecessary variability in advective flows for the simulations of consolidation-induced solute transport (Section 5.3). Close agreement for the other settlement data points (i.e., other than final settlement) suggests that the hydraulic conductivity constitutive relationship (Fig. 5.8b) is an accurate approximation for these tests. Simulated pore pressures for normally consolidation conditions are in excellent agreement with regard to both maximum value and rate of decay, whereas simulated pore pressures for overconsolidated conditions (J7) are in less agreement with regard to minimum values, especially during unloading. This discrepancy likely results from the higher stiffness of the soil skeleton and higher friction along the sidewalls of the
Simulated final void ratios are slightly lower than measured values for each test. Numerical simulations for tests J1, J3, and J4, also showed similar close agreement to the experimental measurements. (Appendix C). The overall excellent agreement between measured and simulated data in Figs. 5.9 – 5.11, and in particular the second load increment of J5 (Fig. 5.10), indicates that CST2 is capable of modeling large strain consolidation for the kaolinite specimens tested in this research.
5.3 Solute Transport Data

5.3.1 Solute mass balance

Measurements of solute mass for the solute transport tests are provided in Table 5.3. The experimental error $E$ in solute mass balance for J1, J2, J4, J5, and J6 was evaluated as,

$$E(\%) = \frac{M_f - M_o}{M_o} \times 100 \quad (5.3)$$

where $M_o$ is initial solute mass in the specimen and $M_f$ is sum of final solute mass in the specimen and all solute mass losses due to pore water outflow or reservoir sampling. Mass balance errors for both Br$^-$ and K$^+$ are generally small and indicate that solute mass calculations are accurate to approximately 10%. This also suggests that the nitric acid extraction procedure was effective in desorbing K$^+$ from the solid phase. One contribution to the mass balance errors is the assumption of a linear distribution between measurements in the final solute concentration profiles, whereas the true distributions are expected to follow smooth curves.
<table>
<thead>
<tr>
<th></th>
<th>Br-</th>
<th></th>
<th>K+</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>J1</td>
<td>J2</td>
<td>J3</td>
</tr>
<tr>
<td>$M_o$ (mg)</td>
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<td>-</td>
</tr>
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<td>158.1 $^{d}$ (65.7)$^{c}$</td>
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<td>487.8</td>
<td>485.1</td>
<td>479.3</td>
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- $^{a}$final dissolved solute mass inside specimen
- $^{b}$final sorbed solute mass inside specimen
- $^{c}$total solute mass outflow from specimen (based on measured solute concentration and outflow solute volume calculated from measured settlement)
- $^{d}$final solute mass in reservoir above specimen
- $^{e}$total solute mass removed in reservoir samples
- $^{f}$calculated initial mass using CST2 (based on measure initial water content and solute concentration)

Table 5.3. Solute mass measurements for solute transport tests.
5.3.2 Effect of concentration boundary condition

Measured solute breakthrough curves at the top boundaries of the J1 and J2 specimens are presented in Fig. 5.12. The primary difference for these tests was the top boundary concentration condition (Table 4.3). Simulated breakthrough curves obtained using CST2 are also shown, as are the simulated settlement curves for reference. Fig. 5.12(a) presents solute concentration data, where values for J1 correspond to effluent solute concentration $c_e$ and values for J2 represent reservoir solute concentration $c_{res}$. Breakthrough of both Br$^-$ and K$^+$ occurred during the first load increment. Thereafter, concentrations progressively increased with increasing settlement because larger settlements correspond to greater reductions in void ratio and thus greater advective transport from the contaminated kaolinite layers into the uncontaminated kaolinite layers and out of the specimens. In general, solute concentrations display smooth trends with little dependence on the settlement rate for each load increment. Measured Br$^-$ effluent concentrations for J1 are larger than for J2, which is a consequence of the reservoir dilution effect for J2 (i.e., early effluent to the J2 reservoir was clean). Effluent concentrations for K$^+$ are significantly lower than for Br$^-$ due to lower $c_o$ values and K$^+$ sorption in the uncontaminated layers. By the end of the tests, Br$^-$ concentrations were
approximately 80% of the initial $c_o$ values of the contaminated layers whereas K$^+$ concentrations were approximately 60% of the initial $c_o$ values. Measured K$^+$ concentrations are essentially unaffected by the top boundary concentration condition in these tests.
Fig. 5.12  Breakthrough curves for J1 and J2:  (a) solute concentration, and (b) solute mass.
Fig. 5.12(b) presents solute mass outflow data for the J1 and J2 specimens. Values for J1 \( (M_e) \) are equal to measured effluent concentration \( (c_e) \) multiplied by the incremental effluent volume \( (= \text{incremental settlement} \times \text{area}) \) and thus represent cumulative solute mass outflow. Values for J2 \( (M_{\text{res}}) \) are equal to measured reservoir concentrations \( (c_{\text{res}}) \) multiplied by total reservoir volume \( (= \text{total settlement} \times \text{area}) \) less the volume of samples taken from the reservoir up to that point. Thus, the measured \( M_{\text{res}} \) values match the actual test conditions for J2 but underestimate the cumulative solute mass outflow for this test. All values are presented as percent of initial total solute mass \( (M_o \text{ or } M_{o,\text{CSTZ}}) \) in the contaminated kaolinite layers. Solute mass outflows are in general agreement with the concentration data of Fig. 5.12(a), with cumulative mass increasing with increasing settlement for both tests and ion species. However, unlike Fig. 5.12(a), mass outflow rates show close similarity to the rates of settlement due to the dependence on advection. Faster outflows occur during the early stages of consolidation when pore water outflow rates are high and then slow toward the end of each load increment. Approximately 40% and 6% of the initial masses of \( \text{Br}^- \) and \( \text{K}^+ \), respectively, were expelled from the J1 specimen. Indicated mass outflows from J2 (32% and 8%) are less than true outflows due to sampling effects, which also explains the
decrease of mass outflow after the completion of consolidation for each increment.

Solute concentrations and mass outflows are not proportional in Fig. 5.12 because fluid flow rates are unsteady. As a result, consideration of both types of plots is needed for complete understanding of consolidation-induced transport behavior.

Simulated breakthrough curves for concentration and solute mass are also shown in Fig. 5.12. These simulations were conducted using 200 solid elements, 600 fluid elements, and the required initial, boundary and procedural conditions for each test, including the sampling effects for J2. Excellent agreement with the measured data is observed for both tests and ion species throughout the consolidation process. One additional simulation (J2(ns), i.e., “no sampling”) is shown in which the effects of sampling are ignored and the results thus correspond to cumulative solute mass outflow for J2. A comparison of simulations for J1 and J2(ns) indicates that the reservoir boundary condition for J2 actually produces higher solute mass outflows. J1 corresponds to only advective flux across the top boundary, whereas J2 allows for both advection and diffusion. Thus, the non-zero concentration gradient for the reservoir produces additional diffusive transport that does not occur for J1. At the end of 18 days, the Br⁻ simulations for J1 and J2(ns) indicate 42% and 48% solute mass outflows,
respectively. Corresponding mass outflows for $K^+$ are 6.3% and 9.6% for J1 and J2(ns), respectively. Interestingly, concentration differences between J2 and J2(ns) are relatively small in Fig. 5.12(a).

For clarity, Fig. 5.13 presents the numerical simulations for cumulative mass outflow for J1, J2(ns) and J3, along with simulated settlement curves. The settlement curves are similar for each test, and thus suggest that the transport data should be comparable. The top boundary of J3 was maintained at zero concentration throughout consolidation (Table 4.3) and, as a result, mass outflows could not be measured experimentally. A comparison of simulated results for J1, J2(ns), and J3 indicates the effect of top boundary concentration condition. The zero concentration at the top boundary for J3 substantially increased the total mass outflow of $Br^-$ and $K^+$ as compared to J1 and J2(ns). The numerical simulation for J3 indicated a loss of solute mass of 80% for $Br^-$ and 31% for $K^+$. Corresponding values are 42% and 6.3% for J1 and 48% and 9.6% for J2(ns). To investigate the importance of consolidation on solute transport, Fig. 5.13 includes additional simulation for the J3 initial geometry and diffusion only. For J3 (diffusion), loss of solute mass for $Br^-$ and $K^+$ are 60% and 18%, respectively. For $K^+$, breakthrough starts after $t = 3$ d, which is 2 days later than breakthrough including
consolidation. Fig. 5.13 indicates that boundary concentration condition and consolidation flow are both important factors that affect solute transport for the J3 test.

![Graph showing simulated settlement and cumulative mass outflow for J1, J2(ns), J3, and J3 diffusion only.](image)

**Fig. 5.13.** Simulated settlement and cumulative mass outflow for J1, J2(ns), J3, and J3 diffusion only.
Final measured and simulated fluid concentration profiles for J1, J2, and J3 are shown in Fig. 5.14(a). Simulated profiles for Br$^-$ are in good to excellent agreement with the experimental measurements. All three profiles display a concentration gradient toward the top boundary and a smooth transition between the initially contaminated and uncontaminated layers. Interestingly, final Br$^-$ concentrations are nearly uniform for J1 and equal to approximately 0.85 $c_o$. The J2 profile shows a small decrease in concentration near the top due to the non-zero concentration gradient. The zero concentration at the top boundary for J3 (Table 4.3) produced a strong concentration gradient across the specimen, which is consistent with the higher total mass outflow shown in Fig. 5.13. Simulated profiles for K$^+$ fluid concentrations are in excellent agreement with the experimental measurements. Final sorbed concentration profiles for K$^+$ are shown in Fig. 5.14(b). The trends are consistent with the K$^+$ fluid concentrations in Fig. 5.14(a), which suggests that equilibrium sorption is achieved for these materials.

The numerical simulations are in good agreement for each measured profile. The numerical data in Figs. 5.12 and 5.13 suggest that the CST2 computational model is capable of simulating local flow and transport effects as well as overall solute mass concentrations and outflow masses for the different boundary conditions.
Fig. 5.14. Final concentration profiles for J1, J2, and J3: (a) fluid concentration, and (b) sorbed concentration.
5.3.3 Effect of loading schedule

Measured and simulated solute breakthrough curves for Br\(^-\) and K\(^+\) at the top boundary of the J4 and J5 specimens are shown in Fig. 5.15. The primary difference for these tests was the loading schedule (Table 4.3). Effluent solute concentrations \(c_e\) are presented in Fig. 5.15(a). Similar to Fig. 5.12(a), effluent concentrations increased with increasing settlement. Effluent concentrations increase more quickly for J5 than J4 due to the greater consolidation rate of the J5 specimen. However, the final Br\(^-\) concentration measured for J5 is approximately 60\% of that measured for J4.

Corresponding curves for K\(^+\) indicate much smaller effluent concentrations throughout both tests. Potassium is sorbed to the uncontaminated layer during upward transport and less is carried out of the specimen. The CST2 simulations are in good agreement with Br\(^-\) and K\(^+\) effluent concentrations for both tests.

Plots of dimensionless cumulative solute mass outflows \(\frac{M_e}{M_o}\) for J4 and J5 are presented in Fig. 5.15(b). Data points indicated as “Measurement 1” were calculated based on measured settlements just as with Fig. 5.12(b). The breakthrough curves for solute mass are in general agreement with the effluent concentration curves of Fig. 5.15(a). 34\% of the initial Br\(^-\) mass is transported out of the J4 specimen during
consolidation, whereas only 14% is lost for the J5 specimen. Considering that final settlements (and hence pore water outflows) were almost the same for these tests, it must be concluded that the longer testing time, and hence greater time for diffusion, had a considerable effect on the total solute outflow. The Br⁻ data also show that, similar to Fig. 5.12(b), solute mass outflow rates mimicked the rates of consolidation for the various load increments. Insufficient pore water effluent was collected during secondary compression for analysis, which led to the gaps in the $c_e$ and $M_e/M_o$ curves in Fig. 5.15(b). However, it is presumed that diffusion became more dominant as the advection rate greatly slowed during secondary compression. This diffusion transport resulted in further upward migration of solute mass and the cumulative effect produced the large difference in total Br⁻ mass outflows for J4 and J5 in Fig. 5.15(b). Fig. 5.15(b) also shows that only a small faction (less than 2%) of the initial K⁺ mass was transported out of each specimen, which is due to sorption of this species in the uncontaminated kaolinite layer. The CST2 simulations for mass outflow are again in good agreement with the experimental measurements. The errors in simulated total mass outflows of Br⁻ at the conclusion of J4 and J5 consolidation tests are 3% and 26%, respectively.
Fig. 5.15(b) also shows mass outflow data (“Measurement 2”) for J4 and J5 in which the effluent volume was directly measured (by fluid weight) instead of based on settlement. Due to the small fluid quantities involved (especially for J4), these measurements likely involve more error than the measurements based on settlement. The trend for the “Measurement 2” data points is however similar to the “Measurement 1” points and are in excellent agreement for the K⁺ measurements. This suggests that the calculation of mass outflows based on settlement is reasonable.
Fig. 5.15. Breakthrough curves for J4 and J5: (a) solute concentration, and (b) solute mass.
Final measured and simulated solute concentration profiles for the J4, J5, and J6 specimens are shown in Fig. 5.16. Final heights of the J4, J5, and J6 specimens were 44.1, 44.5, and 73.2 mm, respectively. Bromide fluid concentrations (Fig. 5.16a) for the diffusion test (J6) are lower than for the consolidation tests (J4, J5) even though J6 has the highest initial mass of Br\(^-\) (Table 5.3). This likely occurred due to additional dilution in the larger volume of uncontaminated pore water for this specimen. Some of the uncontaminated pore water was expelled from the J4 and J5 specimens during consolidation and this produced higher final concentrations of Br\(^-\). The J5 profile has a higher average concentration than J4, which is consistent with the breakthrough curves in Fig. 5.15(a). Interestingly, the J5 Br\(^-\) profile also shows a much higher final concentration gradient than the J4 profile. This is likely due to the additional time allowed for diffusion in the J4 test which caused re-distribution of solute mass and produced a final Br\(^-\) profile that more closely resembles a uniform concentration condition. Final profiles for K\(^+\) (Fig. 5.16a) show relatively small fluid concentrations for all three tests due to sorption of K\(^+\) onto the solid phase. The trends of these curves are similar to the Br\(^-\) profiles except that J6 had the highest average concentration. Since only very small quantities of K\(^+\) were transported out of the consolidation
specimens, the higher J6 concentration reflects the higher initial mass $M_o$ in this specimen (Table 5.3).
Fig. 5.16. Final concentration profiles for J4, J5, and J6: (a) fluid concentration, (b) sorbed concentration, (c) normalized fluid concentration profile, (d) normalized sorbed concentration profiles.
Fig. 5.16 continued
Final sorbed concentration profiles for $K^+$ are shown in Fig. 5.16(b). The trends are consistent with the $K^+$ fluid concentrations in Fig. 5.16(a), with all three profiles displaying a concentration gradient toward the top boundary and a smooth transition between the initially contaminated and uncontaminated layers. The effect of differences in final specimen height $H_f$ can be removed by plotting concentration profiles in terms of relative elevation $z/H_f$ (Figs. 5.16c and 5.16d). Interestingly, the $K^+$ fluid and sorbed concentration profiles for J4 and J6 collapse to a single trend in this case, which suggests that diffusion is important for the redistribution of solute mass in J4. Most of the $K^+$ mass for J4 remains inside the specimen throughout consolidation process even though advection increases the rate of $K^+$ transport in the upward direction. Diffusion after the end of each consolidation stage redistributes the solute mass inside the specimen. The data suggest that the final concentration profile is governed by diffusion and, as a result, the $K^+$ fluid and sorbed concentration profiles for J4 and J6 show similar trends if the effect of height differences are eliminated. The J5 test, in which consolidation and diffusion occurred over a much shorter time (6 d), has a higher sorbed concentration gradient. J5 also displays a sorbed concentration at the top that is nearly zero. This is consistent with the very small mass outflow of $K^+$ in Fig. 5.15(b) and Table 5.3. The
CST2 simulations shown in Fig. 5.16 are in again good agreement with the experimental measurements for fluid concentration profiles of Br\(^-\) and K\(^+\) and sorbed concentration profiles of K\(^+\).

5.3.4 Effect of thickness of uncontaminated and contaminated layers

Fig. 5.17(a) presents a comparison of concentration breakthrough curves for J1 and J4. The primary difference for these tests was the thicknesses of the uncontaminated and contaminated kaolinite layers (Table 4.3). As would be expected, effluent concentrations were higher for the specimen with the thicker contaminated layer (J1). The corresponding mass outflow plot (Fig. 5.17b) also indicates higher mass outflow for J1. The uncontaminated layer for J4 was 2.5 times thicker than that for J1 (Table 4.3). Interestingly, the final effluent concentration of Br\(^-\) for J4 was 2.3 times less than that for J1. Measured and simulated final mass outflows of Br\(^-\) for J4 were 3.2 times less than for J1 (Table 5.3), and were thus not as close to proportional. The thicker lower contaminated layer for J1 was closer to the top boundary, which resulted in earlier breakthrough of both Br\(^-\) and K\(^+\). Table 5.3 indicates that final K\(^+\) mass outflow was 8.7 times greater for J1 than J4 because the thinner uncontaminated layer for J1
provided less sorption. In this case study, mass outflow data provides better insight than concentration data for understanding solute transport.
Fig. 5.17. Breakthrough curves for J1 and J4: (a) solute concentration, and (b) solute mass.
5.3.5 Unload/reload consolidation-induced solute transport test

Measured and simulated breakthrough curves and final concentration profiles for J7 are shown in Figs. 5.18 and 5.19. The increase of effluent concentration with settlement (Fig. 5.18a) is similar to the first 5 load increments for J1. During unloading, the top boundary was maintained at zero concentration and concentrations were not measured. It is unknown if any solute mass outflow occurred due to diffusion during the unloading period. With reloading, solute effluent concentrations again started to increase with increasing settlement. The closeness of agreement for the CST2 simulations with the experimental data is considered to be excellent as shown in Fig. 5.18(a).

The simulated mass outflow plot (Fig. 5.18b) includes measured data points from the first loading stage and the reloading stage. First loading stage measured points are reliable with regard to cumulative mass outflow, and show excellent agreement with simulated results. Reloading measured points were plotted assuming no mass outflow during unloading. However, simulated results in Fig. 5.18(b) indicate that this is a poor assumption and that diffusion significantly increases cumulative mass outflow during the unloading stages. The simulations indicate that losses of Br⁻ and K⁺ mass during the
first unloading stage are 30% and 15% of the initial masses, respectively. During
swelling, clean water was drawn into the specimen and this would be expected to reduce
the rate of solute transport out of the specimen. Interestingly, the simulation indicates
that diffusive transport driven by the high concentration gradient was able to overcome
this advection and carry solute mass out of the specimen during unloading. Again, the
mass outflow data generally provides key insight for the understanding of solute transport.

Figure 5.19 presents final measured and simulated fluid and sorbed concentration
profiles. Simulated concentration profiles (Fig. 5.19a) are in good agreement with the
experimental measurements. The zero concentration at the top boundary for J7 during
unloading stages produced a strong concentration gradient across the specimen similar to
J3. The trends of final sorbed concentration profiles for K⁺ (Fig. 5.19b) are consistent
with the K⁺ fluid concentrations (Fig. 5.19a), and the numerical simulations are in good
agreement. Figs. 5.18 and 5.19 indicate that the CST2 computational model can
simulate more complicated consolidation-induced solute transport, which includes
unloading and reloading.
Fig. 5.18  Breakthrough curves for J7:  (a) solute concentration, and (b) solute mass.
Fig. 5.19  Final concentration profiles for J7: (a) fluid concentration, and (b) sorbed concentration.
5.3.6 Effect of nonequilibrium sorption

Figures 5.20 – 21 present the results of additional simulations for J1 that indicate the effects of nonequilibrium sorption on consolidation-induced transport of $K^+$. Concentration breakthrough curves are shown in Fig. 5.20(a) for varying values of sorption rate constant $\lambda$. The initial condition for each simulation was equilibrium sorption in the contaminated kaolinite layer. After consolidation begins, a value of $\lambda = 0$ corresponds to no sorption/desorption (i.e., $s = \text{constant}$) and $\lambda = \infty$ corresponds to equilibrium sorption/desorption in both layers. The value of $\lambda = 0.005/s$ was based on results of kinetic batch tests (Fig. 5.1b) and was used for all previous transport simulations. Effluent concentrations are highest for $\lambda = 0$ because no sorption occurs in the uncontaminated kaolinite layer and then decrease as $\lambda$ increases. Curves for $\lambda = 0.005/s$ and $\lambda = \infty$ are virtually identical and are in closest agreement with the experimental data. This suggests that equilibrium sorption conditions were essentially achieved in the J1 test. Fig. 5.20(a) also shows interesting undulations of effluent concentration for intermediate values of $\lambda$. These undulations occur due to time-dependent sorption in the uncontaminated layer, which becomes more effective in reducing $c_e$ as the advection rate decreases for each load increment. Simulated solute mass outflows (Fig. 5.20b) progressively decrease with increasing $\lambda$ and also suggest that equilibrium conditions were achieved for J1.

Final fluid and sorbed concentration profiles for $K^+$ are shown in Fig. 5.21. As $\lambda$ increases, fluid concentrations in the initially uncontaminated layer first decrease due to higher sorption and then increase, which is presumably due to higher desorption in the contaminated layer below. In the initially contaminated layer, fluid concentrations
consistently decrease with increasing $\lambda$. Sorbed concentration profiles are discontinuous for low $\lambda$ and gradually become smooth as sorption approaches equilibrium. Simulations for $\lambda = 0$ and 0.005/s are again virtually identical and in closest agreement with the experimental measurements. Corresponding data and simulations for J5 also indicate that equilibrium sorption was nearly achieved (Fig. 5.22). Thus, for these materials and test conditions, the experimental data suggest that kinetic sorption effects were not significant and the assumption of equilibrium sorption is valid.
Fig. 5.20  Effect of sorption rate constant on breakthrough curves for J1: (a) solute concentration, and (b) solute mass
Fig. 5.21  Effect of sorption rate constant on final concentration profiles for J1: (a) fluid concentration, and (b) sorbed concentration
Fig. 5.22 Effect of sorption rate constant on breakthrough curves and final concentration profiles for J5: (a) solute concentration, (b) solute mass, (c) fluid concentration, and (d) sorbed concentration
Fig. 5.22 continued
5.4 Further Experimental Verification for CST2 Model

Experimental and numerical results in terms of concentration for each solute transport test are represented in Appendix D. Corresponding cumulative mass outflows and final measured and simulated solute mass profiles for each solute transport test are presented in Appendix E. Measured mass profiles were obtained from the volume of sliced horizontal disks after solute transport tests, and mass profiles using CST2 were also calculated based on the measured volume of the disks. Each horizontal disk has slightly different height (i.e., volume), thus both the measured and the calculated mass profiles are irregular in these plots. However, they provide enough data points to validate numerical simulations, and indicate that the experimental and numerical results are generally in excellent agreement.
CHAPTER 6

CONCLUSIONS AND RECOMMENDATIONS

The following conclusions are reached as a result of: 1) the development of the CST2 numerical model and subsequent investigation of the importance of variable effective diffusion coefficient and nonlinear nonequilibrium sorption for consolidation-induced solute transport, 2) the experimental investigation of the effect of clay consolidation on parameters governing the advective-dispersive transport of a dilute inorganic solute, and 3) the experimental and numerical investigation of consolidation-induced solute transport.
6.1 CST2 Numerical Model for Consolidation-Induced Solute Transport with Nonlinear and Nonequilibrium Sorption

1. CST2 is a numerical model for consolidation-induced solute transport that represents the next level of sophistication beyond the model CST1 (Fox 2007a, 2007b). CST2 was developed using a dual-Lagrangian framework that separately follows the motions of fluid and solid phases. The consolidation algorithm accounts for large strains with associated geometric and material nonlinearities. The transport algorithm accounts for advection, dispersion, and sorption, and includes variation of effective diffusion coefficient during consolidation and nonlinear nonequilibrium sorption effects.

2. Verification checks of CST2 were performed for solute transport through rigid porous media with a spatially varying effective diffusion coefficient, nonlinear equilibrium sorption, and linear nonequilibrium sorption. Simulations were also conducted for diffusion transport with a reservoir boundary condition. Breakthrough curves and concentration profiles are in excellent agreement with existing analytical and numerical solutions for several test cases.

3. A parametric study was conducted on solute transport for a hypothetical single-increment consolidation test. The clay slurry specimen consisted of a thin
uncontaminated layer overlying a thicker contaminated layer and a reservoir top boundary condition. For the conditions considered, variation of effective diffusion coefficient during consolidation had an important effect on solute transport, whereas nonlinearity of the sorption isotherm had a less important effect. Additional simulations showed that nonequilibrium (i.e., kinetic) sorption can have a strong effect on consolidation-induced solute transport and that this effect becomes more important as the rate of consolidation increases. The simulations in this study corroborate the findings of Fox (2007b) that consolidation can have a lasting effect on solute migration because transient advective flows change the distribution of solute mass within the specimen which then becomes the initial condition for subsequent transport processes.
6.2 Effect of Clay Consolidation on Solute Transport Parameters

1. Batch, diffusion, and dispersion column tests were conducted on specimens of kaolinite to assess the effect of changing void ratio on transport parameters for potassium bromide (KBr). Bromide (Br\textsuperscript{-}) served as a nonreactive tracer for these tests, whereas potassium (K\textsuperscript{+}) experienced sorption according to a nonlinear (Freundlich) isotherm. Kinetic batch tests indicated that equilibrium K\textsuperscript{+} sorption occurred within approximately 30 min.

2. Batch tests produced higher levels of K\textsuperscript{+} sorption than the consolidation or dispersion column tests. This is presumably due to the lower solids-to-solution ratio and more efficient mixing that occurs for batch tests. Kaolinite consolidation had little effect on the sorption isotherm for K\textsuperscript{+}.

3. The effective diffusion coefficient (\(D^*\)) for both Br\textsuperscript{-} and K\textsuperscript{+} decreased with decreasing porosity. \(D^*\) values for Br\textsuperscript{-} were generally larger than values for K\textsuperscript{+}. When plotted in terms of apparent tortuosity factor (i.e., \(D^*/D_o\), where \(D_o\) = free solution diffusion coefficient), the data are well described by a single nonlinear relationship.
4. Transport parameters obtained from the dispersion column tests were strongly
dependent on method of analysis. The analysis method using resident
concentrations and semi-infinite boundary conditions (Method I) produced the closest
agreement between calculated isotherms for $K^+$ and corresponding isotherms
measured from batch and consolidation tests. The hydrodynamic dispersion
coefficient ($D_h$) for both $Br^-$ and $K^+$ decreased with decreasing porosity. $D_h$ values
for $K^+$ were significantly larger than values for $Br^-$. 

5. Values of longitudinal dispersivity ($\alpha$) were larger for $K^+$ than $Br^-$, which results
primarily from differences in the respective $D_h$ values. Dispersivity showed no
clear trend with decreasing void ratio.

6. In general, changes in $D^*$ and $D_h$ should be taken into account during clay
consolidation whereas sorption isotherm and $\alpha$ may be considered as unchanged
during the consolidation process.
6.3 Experimental and Numerical Investigation of Consolidation-Induced Solute Transport

1. Solute transport tests were conducted on composite specimens of kaolinite to investigate the effect of media consolidation on solute transport and to validate the CST2 numerical model. The solute transport tests consisted of one diffusion test (J6) and six consolidation-induced solute transport tests (J1 – J5, and J7). Experimental data and numerical simulations were presented with respect to various boundary conditions (J1 – J3), different loading schedules (J4 – J6), different thickness combinations (J1 and J4), and consolidation-induced solute transport that included unloading and reloading effects (J7).

2. Experimental data for J1, J2, and J3 showed that consolidation-induced solute transport is significantly affected by boundary concentration condition. Loss of solute mass for J2 was unavoidable due to reservoir sampling, but CST2 simulations that included this sampling effect showed an excellent agreement with experimental results. Simulation for J2(ns) that did not include the sampling effect showed that cumulative solute mass outflows would have been higher for J2 than J1 if sampling had not occurred. This results from the additional diffusive transport driven by a non-zero concentration gradient at the top.
boundary of the J2 specimen. Furthermore, measured and simulated results for J3 showed that zero concentration at the top boundary produces the greatest mass outflow and the lowest concentration profiles due to diffusive transport. The experimental and numerical results confirm the findings of Alshawabkeh et al. (2004) that consolidation accelerates solute transport if advection is in the same direction as the concentration gradient.

3. A diffusion test (J6) and two consolidation-induced transport tests (J4 and J5) were performed to investigate the importance of loading schedule. J6 involved no advection and produced final profiles of Br\(^-\) and K\(^+\) that indicated considerable redistribution of solute mass over the 18 d diffusion period. The consolidation-induced solute transport tests produced significant outflows of Br\(^-\) solute mass in response to specimen consolidation. Effluent concentrations increase more quickly for J5 than J4 due to the greater consolidation rate of the J5 specimen. Outflows of K\(^+\) were much less due to sorption in the initially uncontaminated layer. When compared to the diffusion test, transient advective flows caused by consolidation had a significant effect on solute breakthrough and final distribution of solute mass within the specimens.
4. The effect of thickness of uncontaminated and contaminated layers for the composite specimens was also found to be an important factor. In these experiments, a thinner overlying uncontaminated layer resulted in faster breakthrough and higher effluent concentrations. Experimental results indicated that the thickness of the uncontaminated layer was more important for a reactive ion ($K^+$) than a nonreactive ion ($Br^-$) due to sorption.

5. Consideration of both concentration and solute mass data is necessary to gain a complete understanding of consolidation-induced solute transport behavior because advection rates are unsteady and void ratio can vary over the height of the specimen.

6. Depending on initial and concentration boundary conditions, the results indicate that diffusion, in addition to advection, can also play an important role in consolidation-induced solute transport.

7. This limited testing program has indicated that neglecting to consider transient consolidation effects may lead to serious errors in transport analyses for soft contaminated clays undergoing large strain consolidation.

8. Numerical simulations obtained using the CST2 model were in good to excellent
agreement with all experimental measurements in this research program. Comparisons were made based on solute breakthrough and final concentration profiles of both solute concentration (fluid and sorbed) and solute mass, and included solute transport tests conducted for different initial, boundary, and loading conditions (including unload/reload effects). This suggests that the CST2 computational model is capable of simulating local flow and transport effects as well as overall solute mass outflow and mass profiles for consolidation-induced transport of both tracer and reactive contaminant species.
6.4 Recommendations for Future Study

The following topics are recommended for future study:

1. The CST2 model can assist in the evaluation of the most efficient and cost effective means to remediate contaminated sediments, such as in-situ capping vs. dredging and disposal in a confined disposal facility, possibly including reactive (i.e., sorptive) layers in either design.

2. A model based on CST2 and including more general sorption isotherms can be developed. Two-site kinetic sorption models are widely used to simulate contaminant transport during remediation, so the incorporation of two-site sorption would be a useful enhancement of CST2.

3. Geotechnical centrifuge tests have been performed to model consolidation-induced solute transport, but there has been no rigorous numerical model to simulate the experimental results. A piecewise-linear centrifuge consolidation model called CC1 (Fox et al. 2005) can be easily accommodated in CST2 for the simulation of these effects. More extensive experimental investigations would also be needed to validate a such a model.

4. It should be possible to modify CST2 to investigate solute transport through a
clay membrane barrier (Malusis and Shackelford 2004). Currently available models are developed based on steady-state chemico-osmotic flow conditions, but there is volume change caused by chemico-osmotic consolidation. Therefore, accuracy of simulations can be improved if transient advective flows caused by chemico-osmotic consolidation are more correctly modeled.
LIST OF REFERENCES


APPENDIX A

DISPERISON COLUMN TEST RESULTS
Fig. A.1  Measured and simulated breakthrough curves for D2 test

Fig. A.2  Measured and simulated breakthrough curves for D4 test
Fig. A.3  Measured and simulated breakthrough curves for D5 test

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Table A.1  Measure void ratio (porosity) profiles for dispersion column tests
APPENDIX B

DIFFUSION COLUMN TEST RESULTS
Fig. B.1  Measured and simulated curves for C2 test

Fig. B.2  Measured and simulated curves for C3 test


**Fig. B.3** Measured and simulated curves for C4 test

**Fig. B.4** Measured and simulated curves for C5 test
Fig. B.5  Measured and simulated curves for C6 test

Fig. B.6  Measured and simulated curves for C7 test
Fig. B.7  Measured and simulated curves for C8 test

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Table B.1  Measure void ratio (porosity) profiles for diffusion column tests
APPENDIX C

CONSOLIDATION TEST RESULTS
Fig. C.1 Experimental data and numerical simulations for J1: (a) settlement,
(b) pore pressure, and (c) final void ratio.
Fig. C.1 continued

![Graph showing void ratio (e) versus elevation (z) with symbols for measurement and line for CST2 model.](image)
Fig. C.2  Experimental data and numerical simulations for J3: (a) settlement,
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Fig. C.2 continued
Fig. C.3  Experimental data and numerical simulations for J4: (a) settlement, (b) pore pressure, and (c) final void ratio.
Fig. C.3 continued
APPENDIX D

SOLUTE TRANSPORT TEST RESULTS

(CONCENTRATION)
Fig. D.1 Experimental and numerical results for J1: (a) breakthrough curve, (b) final fluid profile, and (c) sorbed profile.
Fig. D.1 continued

- **Sorbed Concentration, \( s \) (mg/kg)**
- **Elevation, \( z \) (mm)**

- **Measured**
- **CST2**
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Fig. D.2 continued
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Fig. D.4  Experimental and numerical results for J4: (a) breakthrough curve, (b) final fluid profile, and (c) sorbed profile.
Fig. D.4 continued

![Graph showing measured and modelled sorbed concentrations vs elevation. The graph plots elevation (z) on the y-axis and sorbed concentration (s) on the x-axis. The x-axis ranges from 0 to 400 mg/kg, and the y-axis ranges from 0 to 50 mm. The graph includes a black line labeled 'CST2' and a line of data points labeled 'Measured'.]
Fig. D.5  Experimental and numerical results for J5: (a) breakthrough curve, (b) final fluid profile, and (c) sorbed profile.
Fig. D.5 continued

Elevation, $z$ (mm)

Sorbed Concentration, $s$ (mg/kg)

Measured

CST2
Fig. D.6  Experimental and numerical results for J6:

(a) final fluid profile and (b) sorbed profile.
Fig. D.7  Experimental and numerical results for J7: (a) breakthrough curve,
(b) final fluid profile, and (c) sorbed profile.
Fig. D.7 continued

![Graph showing sorbed concentration vs. elevation. The graph has data points and a curve labeled CST2, representing the measured sorbed concentration.]
APPENDIX E

SOLUTE TRANSPORT TEST RESULTS

(MASS)
Fig. E.1  Experimental and numerical results for J1: (a) breakthrough curve, (b) final fluid profile, and (c) sorbed profile.
Fig. E.1 continued
Fig. E.2  Experimental and numerical results for J2: (a) breakthrough curve,
(b) final fluid profile, and (c) sorbed profile.
Fig. E.2 continued
Fig. E.3  Experimental and numerical results for J3:

(a) final fluid profile and (b) sorbed profile.
Fig. E.4  Experimental and numerical results for J4: (a) breakthrough curve, (b) final fluid profile, and (c) sorbed profile.
Fig. E.4 continued

Elevation, $z$ (mm) vs. Sorbed Mass, $M_s$ (mg)

- Measured
- CST2

Measured data points are shown as circles, and the CST2 line is represented by a solid line.
Fig. E.5  Experimental and numerical results for J5: (a) breakthrough curve, (b) final fluid profile, and (c) sorbed profile.
Fig. E.5 continued
Fig. E.6  Experimental and numerical results for J6:

(a) final fluid profile and (b) sorbed profile.
Fig. E.7  Experimental and numerical results for J7: (a) breakthrough curve, (b) final fluid profile, and (c) sorbed profile.
Fig. E.7 continued

![Graph showing Elevation, z (mm) vs. Sorbed Mass, $M_s$ (mg)](image)

- **Measured**
- **CST2**

- Elevation, $z$ (mm)
- Sorbed Mass, $M_s$ (mg)