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Numerical analysis of drying process of soils using finite volume method

Xiaojun Li [a,*], Kun Zhang [b]

[a] Dept. of Civil & Geomatics Engineering, Lyles College of Engineering, California State University, Fresno, 2320 E. San Ramon Ave., M/S EE94, Fresno, CA 93740-8030, United States

[b] Department of Civil and Environmental Engineering, Washington State University, Spokane Street, Sloan Hall 26, Pullman, WA 99164, United States

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Abstract

The accurate prediction of the moisture content in soil is important for pavement engineering. The MEPDG uses the Enhanced Integrated Climate Model (EICM) to consider the effects of environment on the moisture contents of unbound and subgrade soil using models related to unsaturated hydraulic conductivity. These models are mostly empirical and not applicable to relatively dry conditions. This is because at relatively dry condition, the moisture in the pore structure of the soil is not inter-connected. Therefore, the moisture diffusion in porous material controls the moisture migration. When the diffusion coefficient is a nonlinear function of pore relative humidity (RH), there is no closed-form solution of the constitutive differential equation of the moisture diffusion. This study used finite-volume method (FVM) and finite-element method (FEM) for the numerical simulation of the moisture diffusion in soils. The FVM, which is similar to the FEM, uses small and finite-sized elements for simulation, but is based on the law of conservation. Therefore, FVM will be more suitable for flux conservation problems such as moisture diffusion. The FVM results were verified with laboratory experiments and compared with FEM results. The results indicate the applicability of using FVM in the simulation of the moisture migration in soils.

Keywords: Finite volume method (FVM); Numerical analysis; Moisture diffusion; Soil

1. Introduction

In pavement engineering, it's generally accepted that the moisture variation can cause significant variation of the mechanical properties of soils and treated soils, which are commonly used as subgrade, subbase, and base layers. These mechanical properties include modulus, strength, stiffness, as well as deformation properties [1,2]. The Mechanistic-Empirical Pavement Design Guide (MEPDG) and the associated AASHTOWare software Pavement ME use the Enhanced Integrated Climate Model (EICM) to consider the effects of environment on the moisture contents of unbound and subgrade soil. In this process, an unsaturated hydraulic conductivity based on the soil water characteristic curve (SWCC) proposed by Fredlund et al. was incorporated [3]. After the moisture contents are predicted, the resilient modulus adjustment factors at different moisture levels from reference condition (normally at or near the optimum water content) are calculated using embedded model as shown in Eq. (1) [4].

$$logF_u = a + \frac{b-a}{1 + EXP\left[ln\left(-\frac{b}{a}\right) + k_m\left(s - s_{opt}\right)\right]} \tag{1}$$

where F_u is resilient modulus adjustment factor, a, b, and k_m are regression parameter, S is the predicted degree of saturation from EICM, and S_{opt} is the degree of saturation at maximum dry density and optimum moisture content in decimal.

* Corresponding author.
E-mail addresses: xli@csufresno.edu (X. Li), kun.zhang2@wsu.edu (K. Zhang).
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However, these models are mostly empirical and not applicable to relatively dry conditions, such as 30% below S_{opt} [4]. This is because at relatively dry conditions, the moisture in the pore structure of the soil is not interconnected. In this case, the moisture diffusion in porous material controls the moisture migration. However, based on a study on the moisture content of unbound layers of 10 LTPP-SMP sites, most of the base and subbase materials are usually at very low degrees of saturation, typically 50% lower than S_{opt} [4]. Therefore it is important to model and predict the moisture migration and moisture loss in soil at relatively dry condition. The modeling and prediction of moisture migration and moisture loss is also closely related with shrinkage and cracking of pavement layers, which can cause loss of structural integrity and the infiltration or seepage of water into the material and lead to severe engineering problems, such as erosion, weakness of foundation, and reflective cracking [5].

The moisture loss depends on the surface area, the lengths of the moisture migration pathways, and the drying environment [6]. It also depends on the material property, such as diffusion coefficient. Based on the work conducted by Bazant and Najjar [7], the moisture diffusion in porous materials can be characterized by moisture flux, J, which denotes the mass of the water that passes through a unit area that is perpendicular to moisture flux J, within a unit time interval. Moisture flux, J, can be expressed in two different ways. It can be defined in terms of the pore relative humidity (RH) gradient or in terms of the evaporable water content gradient [8], as:

$$J = -D\ grad\ (RH) \tag{2}$$

$$J = -D\ grad\ (w_e) \tag{3}$$

where J is the moisture flux; D is the diffusion coefficient corresponding to either pore RH or evaporable water content; RH is the pore relative humidity which is the ratio of the vapor pressure over the vapor pressure at saturation; and w_e is the evaporable water content.

Nonlinear moisture diffusion theory is commonly used to describe the drying process in porous materials. The constitutive differential equation of the moisture diffusion at constant temperature could be expressed as [7]:

$$\frac{\partial RH}{\partial t} = div(D\ gradRH) \tag{4}$$

where RH is the pore relative humidity; D is the diffusion coefficient which is the function of RH.

When the diffusion coefficient D is a constant, there is a closed-form solution of the constitutive differential equation. However, for soils, the diffusion coefficient D is actually not a constant but a function of pore RH or moisture content of the soils [8–12]. In this case, Eq. (4) can only be solved numerically.

Due to the nonlinear moisture diffusion and the significant variation of the mechanical properties (including the diffusion coefficient) with the changes of the moisture content, the modeling and prediction of the moisture migration and moisture loss in soil is challenging. Without significant simplification and sacrifice of accuracy, there are no closed-form solutions for the calculation and prediction of the pore RH. Typically, finite-difference method (FDM) and finite-element method (FEM) could be used for numerical solutions. FEM has been used for the numerical simulation of moisture migration within porous materials like soils [2,13]. However, the FDM and FEM have difficulties to handle discontinuities and the mass or energy is not strictly conservative in FDM and FEM simulation [14]. Finite-volume method (FVM) is an alternative, which is similar to FDM and FEM using very small and finite-sized elements for simulation, but based on the law of conservation. Therefore, FVM will be more suitable for flux conservation problems, such as thermal flux or moisture flux.

Few studies have been reported on the simulation of moisture migration within soil using FVM. Therefore, the objectives of this study are: (1) to develop numerical models for the moisture migration, (2) to use FVM as a numerical method for the solution of the developed models, and (3) to verify the FVM simulation results via experiments. Moreover, the models and FVM analysis have the potential to be incorporated in the MPEDG to enhance the moisture prediction and the prediction of the shrinkage related distresses.

2. Models development and experiment Validation plan

2.1. Drying model and FVM simulation

The governing differential equation of the one-dimensional moisture diffusion in terms of pore RH can be written as [15]:

$$\frac{\partial(RH)}{\partial t} = \frac{\partial}{\partial x}\left(D(RH)\frac{\partial RH}{\partial x}\right) \tag{5}$$

where RH is the pore relative humidity; D(RH) is the diffusion coefficient with respect to the pore RH; t is the drying time; and x is the distance from the drying surface.

The diffusion coefficient D(RH) in Eq. (5) can be expressed as a nonlinear function of pore RH, as shown [2,12]:

$$D(RH) = D_0 + c\left(\frac{RH}{1-RH}\right)^d \tag{6}$$

where D_0, c, and d are the regression parameters from diffusion coefficient test. Details of the laboratory test method of diffusion coefficient can be found in references [2,15].

The FVM is used to implicitly solve the one-dimensional moisture diffusion constitutive differential equation by integrating the left and right sides of Eq. (5) over time and volume. The left side is derived as:

$$A = \int_{t}^{t+\Delta t}\int_{x}^{x+\Delta x} \frac{\partial(RH)}{\partial t} dxdt = \int_{t}^{t+\Delta t} \frac{\partial(RH)}{\partial t}\Delta x dt$$
$$= \int_{t}^{t+\Delta t} \partial(RH)\Delta x = \left(RH_p^1 - RH_p^0\right)\Delta x \tag{7}$$

where RH_p^0 is the relative humidity at the cell p and the current time t; RH_p^1 is the relative humidity at the cell p and time of $t+\Delta t$; and Δx is the length of one discretized cell, as shown in Fig. 1.

The right side of Eq. (5) is integrated over time and volume implicitly as:

$$B = \int_{t}^{t+\Delta t}\int_{x}^{x+\Delta x} \frac{\partial}{\partial x}\left(D(RH)\frac{\partial RH}{\partial x}\right) dxdt$$
$$= \left(D\left(RH_E^1\right)\frac{RH_E^1 - RH_P^1}{\Delta x} + D\left(RH_W^1\right)\frac{RH_W^1 - RH_P^1}{\Delta x}\right)\Delta t \tag{8}$$

where RH_P^1, RH_E^1, and RH_W^1 are relative humility in the present cell [(P(i)], east cell [E(i + 1)], and west cell [W(i − 1)] at the time of $t+\Delta t$; $D\left(RH_E^1\right)$ and $D\left(RH_W^1\right)$ are the diffusion coefficients at the east cell and west cell depending on their relative humidity at the time of $t+\Delta t$, and can be written as $D\left(RH_E^1\right) = D_0 + c\left(\frac{RH_E^1}{1-RH_E^1}\right)^d$, $D\left(RH_W^1\right) = D_0 + c\left(\frac{RH_W^1}{1-RH_W^1}\right)^d$.

Based on Eqs. (5), (7), and (8), the numerical algorithm for the moisture diffusion in the soil becomes:

$$\left(RH_p^1 - RH_p^0\right)\Delta x = \left(D\left(RH_E^1\right)\frac{RH_E^1 - RH_P^1}{\Delta x} + D\left(RH_W^1\right)\frac{RH_W^1 - RH_P^1}{\Delta x}\right)\Delta t \tag{9}$$

The Eq. (9) can be rearranged as:

$$RH_P^1\left(\frac{\Delta x}{\Delta t} + \frac{D\left(RH_E^1\right)}{\Delta x} + \frac{D\left(RH_W^1\right)}{\Delta x}\right)$$
$$= \frac{D\left(RH_E^1\right)}{\Delta x}RH_E^1 + \frac{D\left(RH_W^1\right)}{\Delta x}RH_W^1 + RH_P^0\frac{\Delta x}{\Delta t} \tag{10}$$

The derived Eq. (10) is solved using the Tridiagonal Matrix Algorithm (TDMA) method.

2.2. Experiment Validation of FVM simulation

The FVM code was developed using Matlab (R2017a). The FVM simulation needs to measure the material parameters in the aforementioned models. Two types of soils were used in this study: a silty clayey sand from Pullman, Washington and a clay from Madison, Wisconsin. The primary properties and grain size distributions of the two types of soils are shown in Table 1 and Fig. 2, respectively.

The material parameters in Eq. (6) measured in the laboratory for diffusion coefficient modeling are given in Table 2. Details of the laboratory measurements can be found in Refs. [2,15]

Laboratory tests were designed in order to experimentally verify the FVM simulation results. In this verification test, a cuboid specimen with length of 285 mm and cross-section of 100 mm by 100 mm was used. All surfaces of the specimen were sealed with wax except at one end for one-dimensional drying test. The specimens were kept in a controlled ambient RH and at 20 °C for several days. After the specimens were dried for 5, 10, or 20 days, they were slice-cut to measure the gravimetric moisture content of each slice, as shown in Fig. 3. At each drying day, the average of two replicates was reported and presented in this study. The gravimetric moisture content could be converted into pore RH through humidity isotherm test results of the silty clayey sand and clay used in this study [2]. The humidity isotherm is a unique correlation between the gravimetric moisture content and the pore RH for each

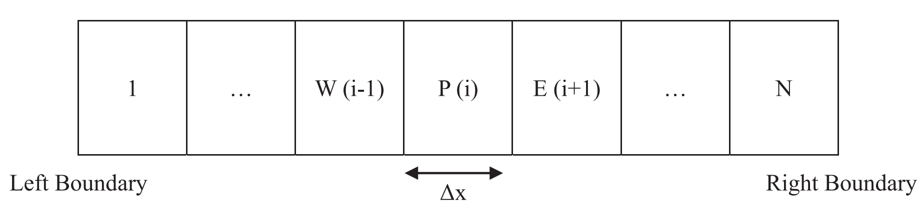

Fig. 1. Schematic of FVM simulation.

Table 1
Properties of the silty clayey sand and clay used in this study.

Soil type	USCS classification	AASHTO classification	Liquid limit	Plastic index	Optimum moisture content (%)	Maximum dry density (g/cm^3)	Specific gravity
Silty Clayey Sand	SM	A-2-4	33	6	11.6	1.93	2.65
Clay	CL	A-6	39	16	19.1	1.72	2.68

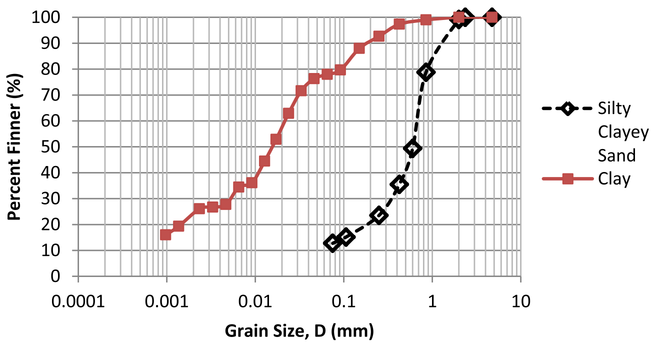

Fig. 2. Grain size distributions of the silty clayey sand and clay used in this study.

Table 2
Material parameters used in diffusion coefficient modeling [Eq. (6)] and FVM simulation.

Material parameter	Silty clayey sand	Clay
D_o	0.856	0.520
c	0.435	0.264
d	1.027	1.027

type of soil. Therefore, the pore RH gradient after the specimens were dried for 5, 10, and 20 days could be obtained.

FVM was used for the simulation of the above laboratory tests, the total simulated time is 20 days with Δt set as 1 h. The total length of the simulated soil specimen is 285 mm with Δx as 1 mm. The boundary condition at the moisture loss surface is defined to equal the ambient RH. At any sealed surfaces without moisture loss, the boundary is defined as $D(\mathrm{RH}_{\mathrm{NE}}^{1}) = 0$. In terms of the initial condition, the RH of all cells is assigned as 99.99% to avoid infinite value of $D(\mathrm{RH})$ as expressed in Eq. (6). The laboratory measured pore RH gradient at 5, 10, and 20 days were used to compare with the FVM simulation results to verify the accuracy of numerical modeling.

3. Results and discussion

After moisture migration for 5, 10, and 20 days, a comparison of the pore RH distributions of the FVM simulation results and the experiment results of the silty clayey sand and clay used in this study are shown in Figs. 4 and 5. It should be noted that, for silty clayey sand laboratory experiments, a constant ambient RH of 60% was controlled and also used in FVM simulation. For clay laboratory experiments, variable natural ambient RH was recorded and used for the FVM simulation. Figs. 4 and 5 indicate a reasonable model prediction and numerical simulation results.

The FVM results in Figs. 4 and 5 were compared with finite element method (FEM) results obtained using program ADINA as well. The FEM simulation procedure is similar as the FVM procedure and available in Refs. [2,15]. It can be seen that, for silty clayey sand, the FVM results are closer to the experiment results than the FEM

Fig. 3. Pore RH simulation validation test.

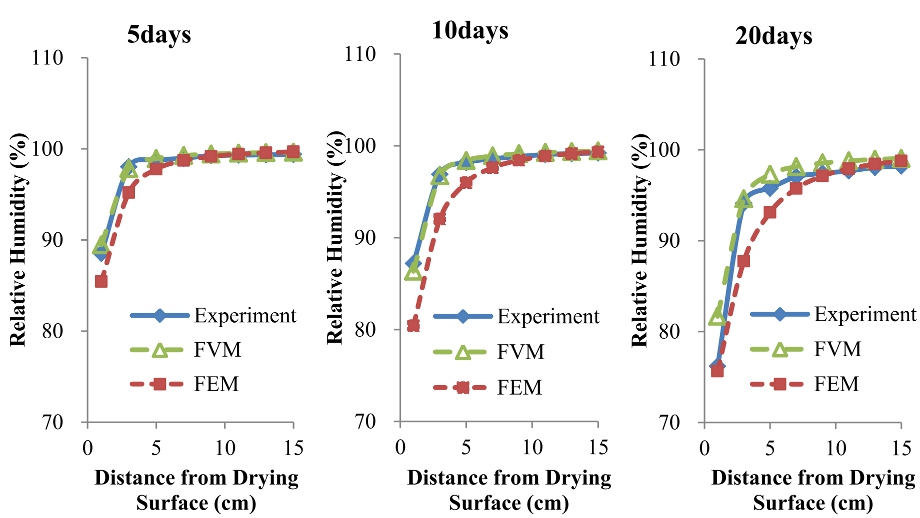

Fig. 4. Comparison of FVM, FEM, and experiment obtained pore RH distributions of silty clayey sand at different drying days.

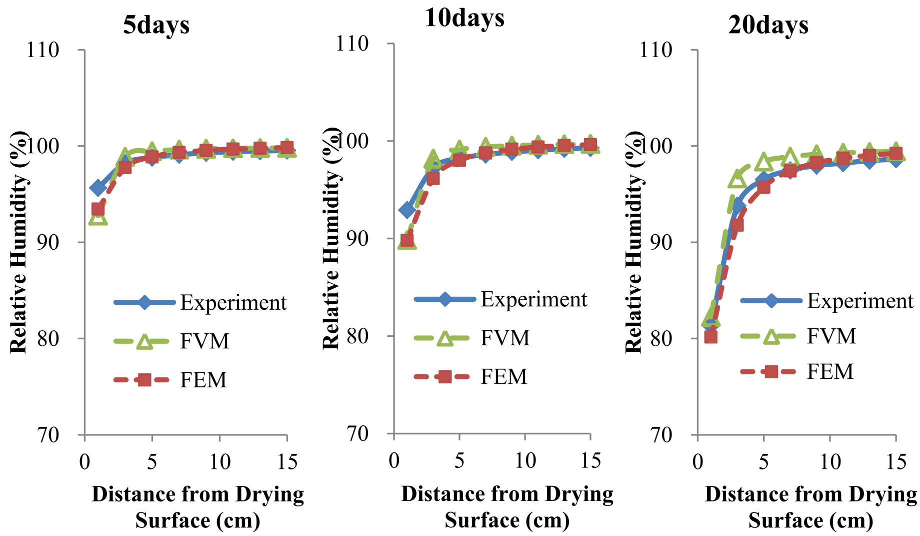

Fig. 5. Comparison of FVM, FEM, and experiment obtained pore RH distributions of clay at different drying days.

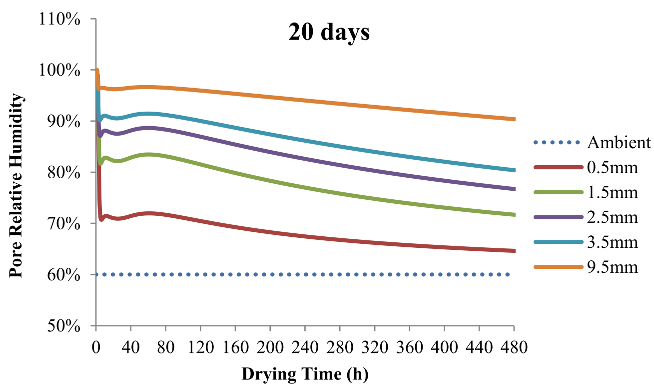

Fig. 6. Pore RH change with drying time at different distance from drying surface for silty clayey sand.

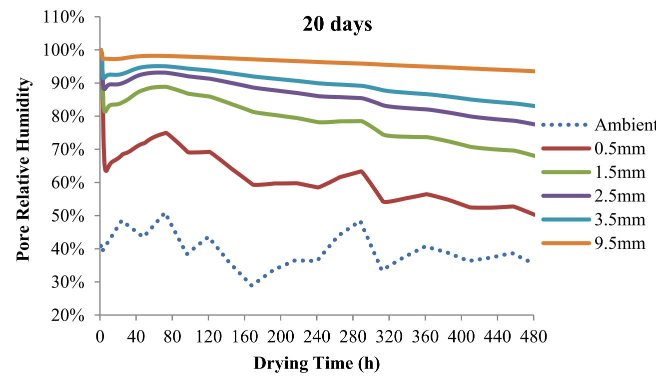

Fig. 8. Pore RH change with drying time at different distance from drying surface for clay.

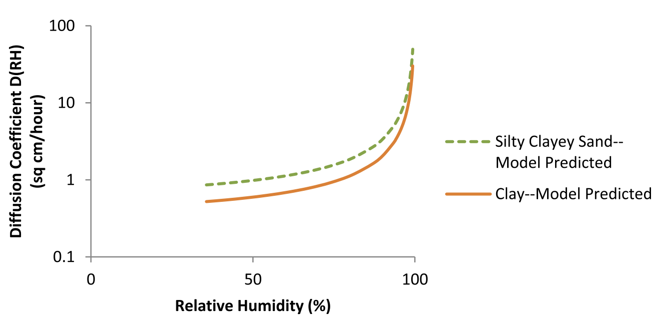

Fig. 7. Plot of diffusion coefficient as a function of pore RH [Eq. (4)].

results. For clay, there is not much difference between FVM and FEM results.

Fig. 6 shows the FVM results in terms of the changes of pore RH at different distances from the drying surface with the time for silty clayey sand. Since the ambient RH is at a constant of 60%, the pore RH at a location very close to surface, i.e., 0.5 mm from drying surface, underwent a quick drop, followed by the small fluctuation, and then decreased slowly but more stable. This is due to the reality that the diffusion coefficient $D(\text{RH})$ as shown in Eq. (6) is a nonlinear function of pore RH. At high pore RH the D (RH) reduced sharply with the reduction in pore RH, as shown by the plot in Fig. 7. At a location close to the drying surface, the diffusion coefficient decreased quickly and faster than the diffusion coefficient at an inner location. This means the moisture at an inner location can move and replenish to the location closer to the drying surface, which causes a fluctuation of the pore RH around 10 to 60 h of drying. This explanation was verified by setting diffusion coefficient as a constant in our FVM simulation, of which the pore RH fluctuation around 10 to 60 h disappeared and the pore RH decreased stably.

Fig. 8 shows the FVM results for the changes of the pore RH at different distances from the drying surface with the time for clay. Since the ambient RH varied in the test of the clay specimen, the pore RH fluctuations due to the change of diffusion coefficient as a function of pore RH in Eq. (6) was obscured by the effect of ambient RH. It can be seen that the pore RH at a location of 0.5 mm from drying surface fluctuates with the ambient RH more significantly than the pore RH at inner locations. At a location of 9.5 mm from the drying surface, the ambient RH variation has little effect on the change of the pore RH. It is also seen that the pore RH may increase depending on the ambient RH, which indicates that the wetting process is also considered in the simulation.

4. Conclusions and recommendations

Accurate prediction of the moisture content in soil is important for pavement engineering. Since the moisture in the pore structure of the soil is not inter-connected at relatively low moisture contents, moisture diffusion controls the moisture migration. For the constitutive differential equation of the moisture diffusion, when the diffusion coefficient is a nonlinear function of the pore RH, numerical method needs to be used for the solutions. The FVM and FEM methods were used in this study for this purpose, and the following conclusions can be made:

(1) The moisture diffusion models in this study could be used for predicting the moisture migration in soils with reasonable accuracy.
(2) Based on the results of the two types of soils used in this study, compared to FEM, FVM results are closer to the laboratory test results for silty clayey sand. For clay, FVM and FEM results show similar accuracy.
(3) When diffusion coefficient is a nonlinear function of pore RH, even under a constant ambient RH, the change in diffusion coefficient can cause fluctuation of the pore RH during drying process. This result shows the importance of accurate characterization and measurement of the diffusion coefficient.

It is recommended that in future study, the 3D models and numerical analysis should be conducted and the effects of temperature and pore size distribution on the moisture migration need to be considered and correlated with model parameters. Typically, FVM modeling uses less computation time, compared with FEM modeling. However, due to the simple scenario in this study, no significant difference in the computation time was observed between these two methods.

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