Title
Development of a discrete-continuum VDFST-CFP numerical model for simulating seawater intrusion to a coastal karst aquifer with a conduit system

Journal
Water Resources Research, 53(1)

ISSN
0043-1397

Authors
Xu, Zexuan
Hu, Bill X

Publication Date
2017

DOI
10.1002/2016wr018758

Peer reviewed

Development of a discrete-continuum VDFST-CFP numerical model for simulating seawater intrusion to a coastal karst aquifer with a conduit system

Zexuan Xu

Bill X. Hu
First published: 22 December 2016
https://doi.org/10.1002/2016WR018758

Abstract

A hybrid discrete-continuum numerical model, Variable-Density Flow and Solute Transport—Conduit Flow Process (VDFST-CFP), is developed to simulate seawater intrusion to a coastal karst aquifer with a conduit network. The Darcy-Weisbach equation is applied to simulate the nonlaminar groundwater flow in the conduit system that is conceptualized as pipes, while the Darcy equation is used for laminar groundwater flow in the continuum porous medium. Density-dependent groundwater flow with appropriate additional density terms in the conduit is analytically derived. The flow and transport equations are coupled, and numerically solved by the finite difference method with an implicit iteration procedure. Two synthetic benchmarks are developed to compare the VDFST-CFP model results with other numerical models, such as the variable-density SEAWAT, constant-density continuum MODFLOW/MT3DMS, and constant-density discrete-continuum CFPv2/UMT3D models. The VDFST-CFP model compares reasonably well with the other model results in both conduit and porous medium domains, and well describes water and salt exchange between the two systems. Under turbulent flow conditions within the conduit, the Darcy-Weisbach equation calculates the flow rate more accurately without overestimation by the Darcy equation. Sensitivity analysis indicates that conduit diameter, friction factor, matrix hydraulic conductivity, and effective medium porosity are important parameters in the VDFST-CFP model. The pros and cons of the VDFST-CFP model are discussed, including the model assumptions and simplifications, limitations of the discrete-continuum modeling method, and the convergence criteria. In general, the newly developed VDFST-CFP model provides a new numerical modeling method for simulating seawater intrusion in a coastal karst aquifer with conduits.

1 Introduction

Karst aquifer systems underlie approximately 10–20% of the Earth's landmass and supply potable water to nearly 25% of the world's population [*Ford and Williams*, 2007]. In the United States, karst aquifers supply almost 52% of all bedrock aquifer withdrawals on a yearly basis [*Maupin and Barber*, 2005; *Covington et al*., 2011]. Karst aquifers are typically characterized by relatively large void spaces and loose porous media, which make the karst aquifers among most productive aquifer systems in the world, for example, the Floridan Aquifer in the United States [*Bush and Johnson*, 1988; *Williams and Kuniansky*, 2015]. The open and porous nature of a karst aquifer, combined with the dissolution of joints and fractures within the bedrocks over time, generate complex subsurface conduit systems and dual-permeability flow regimes [*Davis*, 1996]. Groundwater flow and solute transport processes in conduit networks are generally more rapid than those in the surrounding porous media due to significantly larger hydraulic conductivity and effective porosity of the conduit system [*Ritter et al*., 2002; *Scanlon et al*., 2003]. *Martin and Dean* [2001] pointed out that water and solute interchanges between conduit and porous medium domains are particularly important in a dual-permeability karst aquifer system. As a result, karst aquifers are particularly vulnerable when one considers the problems of groundwater contamination or seawater intrusion [*Arthur et al*., 2007; *Kuniansky*, 2008]. During a high-flow event, contaminants in the conduit system are actively pushed into the carbonate matrix because of the water pressure being higher than that in the matrix. During a low-flow event, contaminants are slowly released from the surrounding porous media into the conduit system, reversing the process [*Martin and Dean*, 1999]. Groundwater contamination and seawater intrusion in a karst aquifer can persist for a long time due to the retention-and-release effect between the conduits and the porous media [*Katz et al*., 2004; *Green et al*., 2006].

Groundwater flow, solute transport, and chemical reactions in a karst aquifer have been studied in a group of laboratory experiments [*Li*, 2004; *Geyer et al*., 2007; *Faulkner et al*., 2009] and numerical simulations [*Lauritzen et al*., 1992; *Groves and Howard*, 1994; *Howard and Groves*, 1995; *Kaufmann and Braun*, 2000]. Groundwater flow and solute transport in a karst aquifer has been simulated by traditional continuum numerical models, with relatively large values of hydraulic conductivity, specific storage, and porosity in the conduit. The hydrological properties and travel times along the conduit network are usually calibrated by the tracer test data and continuous water quality measurements [*Knochenmus and Robinson*, 1996; *Kuniansky et al*., 2001; *Renken et al*., 2005; *Davis et al*., 2010]. The hybrid discrete-continuum numerical model has been developed, tested, and verified as an appropriate approach to simulate groundwater flow and solute transport in a karst aquifer with conduits [*Kiraly*, 1998]. The hybrid model couples the conduit flow in the discrete pipes with Darcian flow in the continuum porous medium. For example, *Clemens et al*. [1996] and *Liedl et al*. [2003] developed the CAVE (Carbonate Aquifer Void Evolution) model based on the hybrid approach. Later, the CFP (Conduit Flow Process) package of MODFLOW-2005 as MODFLOW-CFP was developed by *Shoemaker et al*. [2008] and then has been applied in a number of studies [*Reimann and Hill*, 2009; *Hill et al*., 2010; *Gallegos et al*., 2013]. In recent years, some other modifications and improvements of MODFLOW-CFP were made by *Reimann et al*. [2011a] and by *Reimann et al*.

[2014] to enable the simulations of unsaturated conduit flow, conduit-associated drainable storage (CADS), and time variable boundary condition (TVBC).

In terms of solute transport modeling, MT3DMS is a widely used numerical model that uses the groundwater flow solution from MODFLOW [*Zheng and Wang*, 1999]. Therefore, MT3DMS is only applicable for solute transport with Darcian flow in a porous medium, such as a sandstone or alluvial aquifer. *Spiessl* [2004] and *Spiessl et al*. [2007] modified the MT3D source code and developed RUMT3D (Three-Dimensional Reactive Underground Multispecies Transport), coupled a reactive hybrid transport model with CAVE to simulate solute transport and chemical reactions in a karst aquifer. Furthermore, the coupling of the research version CFPv2 [*Reimann et al*., 2013] and RUMT3D is able to simulate hybrid flow and solute transport (advection and dispersion) in the conduit and porous medium systems under different boundary conditions. In *Xu et al*. [2015a], the coupled CFPv2/UMT3D model was applied to simulate nitrate-N transport in the karst aquifers in the Woodville Karst Plain (WKP), Florida, USA. However, none of the existing hybrid discrete-continuum numerical models has the capability to simulate density-dependent flow, which is critical for modeling seawater intrusion and submarine groundwater discharge in a coastal karst aquifer with conduits.

Seawater intrusion is an important research issue, generating environmental problems globally, such as the salinization of productive soils, localized marine, estuarine ecological changes, and groundwater contamination [*Bear*, 1999]. For example, the subsidence of groundwater level in a coastal aquifer reduces the freshwater hydraulic pressure and allows seawater intrusion to the aquifer, which commonly occurs in urban areas subject to overpumping [*Konikow and Kendy*, 2005; *Chen and Jiao*, 2007]. Buoyancy force associated with the density difference between freshwater and seawater is a major governing factor of the two fluid movements in a coastal aquifer. The Ghyben-Herzberg equation quantitatively states that the position of mixing interface is related to the density of seawater [*Guo and Langevin*, 2002; *Fleury et al*., 2007]. The controlling factors of seawater intrusion into a coastal aquifer system are summarized by *Custodio* [1987] and *Werner et al*. [2013], including the geologic and lithologic heterogeneity, localized surface recharge, paleohydrogeological conditions, climate variations, and anthropogenic influences, all of which play roles in determining salinity distribution in a coastal aquifer. On the other hand, seawater intrusion caused by sea level rise has been recognized as one of the most serious threats to freshwater resources in the world [*Voss and Souza*, 1987; *Bear*, 1999; *IPCC*, 2007; *FitzGerald et al*., 2008]. *Essink et al*. [2010] pointed out that rising sea level, fluctuation of rainfall recharge, and increasing evaporation caused by global climate change will exacerbate the extent of seawater intrusion. According to the Ghyben-

Herzberg relationship, sea level rise brings about severe seawater intrusion in a coastal aquifer, and moves the position of mixing interface significantly landward [*Werner and Simmons*, 2009].

The extensive conduit networks in many coastal karst aquifers are directly open to the sea [*Fleury et al*., 2007]. The complex interchange between conduit and porous media in a karst aquifer is particularly important for seawater intrusion, since the aquifer is particularly vulnerable [*Kuniansky*, 2008; *Davis and Verdi*, 2014]. *Fleury et al*. [2007] reviewed a series of studies on freshwater discharge and seawater intrusion through the intermittent submarine springs and subsurface caves, and concluded that the direction and magnitude of seawater intrusion (or conversely, submarine groundwater discharge) through karst conduits strongly depend on the hydraulic gradient between the aquifer and the sea. The flow pattern at a submarine spring usually exhibits a strong seasonal variation driven by local rainfall conditions [*Arthur et al*., 2007]. Periods of heavy rainfall typically result in large freshwater discharge, which then significantly dilutes the seawater near the submarine springs. During extended low rainfall periods, the hydraulic gradient reverses since a submarine spring no longer acts as a point of freshwater discharge for the local aquifer system, but instead becomes a point of seawater intrusion, which siphons seawater into the underlying conduit system [*Gallegos et al*., 2013; *Davis and Verdi*, 2014]. The Yucatan Peninsula in Mexico is an example of extended seawater intrusion in a coastal karst aquifer, where open sinkholes and submarine springs are widely distributed as passageways for seawater intrusion. Seawater intrusion has been observed to reach tens of miles inland through the highly permeable subsurface layers [*Perry et al*., 2002; *Schmitter-Soto et al*., 2002; *Bauer-Gottwein et al*., 2011]. In addition, evidence shows that seawater intrusion can accelerate the reactive rate of carbonate rock dissolution and porosity change in a karst aquifer [*Sanford and Konikow*, 1989; *Loper et al*., 2005].

Numerical modeling of seawater intrusion is a density-dependent flow issue that involves coupled processes of groundwater flow and salt transport. The transport model is based on the head simulation from groundwater flow model, while salinity determines the groundwater density and affects flow simulation correspondingly. As a result, the mathematical models to couple variable-density flow and transport equations with additional density terms are required. The coupling of flow and transport equations can be solved numerically in either explicit or implicit procedure [*Werner et al*., 2013]. Generally speaking, most variable-density flow and transport coupling models are numerically complicated and computationally expensive, especially when the implicit method is used since flow and transport are calculated multiple times iteratively in each time step until convergence criteria are satisfied [*Guo and Langevin*, 2002; *Werner et al*., 2013]. Several variable-density numerical models have been developed and applied to simulate seawater intrusion processes, including SUTRA [*Voss and Provost*, 1984], in which a finite element and integrated finite difference hybrid methods are applied to solve the mathematical model, and FEFLOW [*Diersch*, 2005], in which a finite element method is used to solve both flow and transport equations. SEAWAT is one of the most popular models for numerical simulation of variable-density groundwater flow and solute transport in a porous medium, in which MODFLOW is used to solve groundwater flow by finite difference method, and MT3D is applied to solve the salt transport by various solution algorithms [*Guo and Langevin*, 2002; *Langevin et al*., 2003]. The variable-density flow equation is solved with appropriate density terms and reformulating the flow equations in terms of fluid mass rather than fluid volume [*Guo and Langevin*, 2002]. However, those density-dependent numerical models only apply to flow in a porous medium, and are not suitable for groundwater flow and salt transport in a karst aquifer with conduits. *Arfib and De Marsily*[2004] developed the SWIKAC (salt-water intrusion in karst conduits) model and numerically simulated the salinity in an inland coastal brackish karstic spring, however, which can only be used to describe groundwater flow and salt transport in a conduit but not in the surrounding porous medium. Many density-dependent benchmark cases, such as Henry and Elder problems [*Henry*, 1964; *Elder*, 1967], have been proposed for numerical modeling of seawater/freshwater mixing in a homogeneous porous medium, but not for a dual-permeability karst aquifer. Recently, *Sebben et al*. [2015] investigated a fractured Henry problem and evaluated seawater mixing processes in a fractured coastal aquifer but not for a karst aquifer with a conduit network.

As mentioned, none of the existing numerical models simulates the variable-density seawater intrusion process in a karst aquifer with conduits. The purpose of this study is to develop a novel hybrid discrete-continuum numerical modeling method to simulate density-dependent groundwater flow and salt transport in both the karst conduit and the porous medium. In the modeling development, the variable-density groundwater flows in the conduit and porous medium are described, respectively, by a discrete pipe flow model and a continuum flow model [*Shoemaker et al*., 2008]. Salt transport in the conduit network and the porous medium is simulated by the advection-dispersion equation. The governing equations are solved by the finite difference method with an implicit iteration procedure. The newly developed discrete-continuum numerical VDFST-CFP model (Variable-density Flow and Solute Transport—Conduit Flow Process) is a physically based numerical model for simulating the interaction of freshwater and seawater in a coastal karst aquifer with a conduit network. In the authors' knowledge, this study is the first attempt to develop a hybrid discrete-continuum numerical model of density-dependent groundwater flow coupled with salt transport.

2 Methods and Governing Equations

The governing equations for variable-density groundwater flow and solute transport in a porous medium are simplified in the VDFST-CFP model, but are similar to other density-dependent numerical models such as SEAWAT [*Guo and Langevin*, 2002] and FEFLOW [*Diersch*, 2005]. The variable-density flow equation for nonlaminar flow within a conduit network is analytically derived to couple with the one-dimensional advection-dispersion transport equation. The coupling technique of flow and transport between conduit and matrix system was proposed by *Spiessl* et al. [2007], and then was applied in many previous studies [*Reimann et al*., 2013, 2014; *Xu et al*., 2015a] and the VDFST-CFP model in this study as well.

2.1 Assumptions

Several assumptions, listed below, are essential in the VDFST-CFP model development to keep the mathematical model conceptually reasonable, and improve the accuracy of numerical model, but significantly decrease the requirements of coding effort, data requirements, and computational cost.

1. The model simulates two-dimensional groundwater flow and salt transport in a porous medium with only one conduit network. The computational cost for three-dimensional spatial domain or multiple conduits is unaffordable for a serial computational model. The large computational cost is mainly due to the implicit iterative procedure, because flow and transport equations have to be solved multiple times iteratively in each time step. The model could be further extended to three-dimensional and multiple conduits in future studies with parallel computing technique for the large computational demanding.
2. The model simulates a confined aquifer with a fully saturated conduit. The groundwater governing equations in a confined aquifer are much simpler than those in an unconfined aquifer with variable thickness and transmissivity. The subsurface conduit system is usually located deep in the coastal karst aquifers: for example, the karst conduit networks in the Woodville Karst Plain (WKP), north Florida, where submarine caves are believed as deep as 300 ft beneath the surface [*Davis*, 1996; *Kernagis et al*., 2008]. In such cases, the calculation complexity of variable saturation in the conduit is not necessary.
3. Groundwater viscosity and water temperature are assumed constant. As a result, density is solely a function of salinity in this study.
4. Effective porosity of the porous medium is assumed constant. The physical and chemical reaction processes that may change the matrix effective porosity, such as carbonate dissolution and precipitation, and weathering and erosion, are not considered in this study.
5. The difference of compressibility coefficients between saline water and freshwater is negligible.
6. The effects of fluid densities on transport modeling are negligible. The solute transport advection-dispersion equation ignores additional density terms, and the effect of variable density only affects groundwater flow modeling.

7. MODFLOW-CFP calculates the Reynolds number of groundwater flow in the conduit, determines whether flow condition is turbulent or laminar, and then applies different equations to calculate flow rate under different conditions [*Shoemaker et al*., 2008]. The simplified Hagen-Poiseuille equation is used in MODFLOW-CFP if the conduit flow is laminar, but is not implemented in the VDFST-CFP model since conduit flow is turbulent in most field cases. Darcy-Weisbach equation is directly applied in the groundwater flow simulation in the conduit, setting aside laminar, or turbulent condition.
8. The dispersion coefficient within the conduit is assumed the same as that in the surrounding porous media. It is difficult to quantify the dispersion coefficient in the conduit network especially under turbulent flow condition.

2.2 Flow Modeling

2.2.1 Variable-Density Groundwater Flow in a Porous Medium

MODFLOW [*McDonald and Harbaugh*, 1988; *Harbaugh et al*., 2000; *Harbaugh*, 2005] applies a continuum Darcy equation to simulate groundwater flow in the aquifer. In this study, the movement of constant density groundwater in the continuum porous medium is studied by a simplified two-dimensional partial differential Darcy equation as follows,

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right)+W=S_s\frac{\partial h}{\partial t} \quad (1)$$

where K_{xx}, K_{zz} are the hydraulic conductivities along *x* and *z* coordinate axes, respectively, which are assumed to be parallel to the major axes of the hydraulic conductivity [L/T]; h is the potentiometric head [L]; W is the volumetric flux per unit volume representing sources and/or sinks of water, with $W < 0.0$ for flow out of the groundwater system, and $W > 0.0$ for flow into the system [T^{-1}]; S_s is the specific storage of the porous material [L^{-1}]; t is the time [T].

The concept of equivalent freshwater head is introduced to simulate variable-density groundwater flow and saline water movement, which is used in the density-dependent SEAWAT model [*Guo and Langevin*, 2002], and in the VDFST-CFP in this study. The conversion between head and equivalent freshwater head can be made using the relationships as follow,

$$h_f=\frac{\rho}{\rho_f}h-\frac{\rho-\rho_f}{\rho_f}Z \quad (2)$$

and

$$h=\frac{\rho_f}{\rho}h+\frac{\rho-\rho_f}{\rho_f}Z \quad (3)$$

where h_f is the equivalent freshwater head [L]; ρ_f is the density of freshwater [ML^{-3}]; ρ is the density of saline groundwater [ML^{-3}]; Z is the elevation [L].

In the variable-density Darcy equation, specific discharges or volumetric fluxes in terms of pressure can be expressed as,

$$q_x = -\frac{k_x}{\mu}\frac{\partial P}{\partial x} \quad (4)$$

$$q_z = -\frac{k_Z}{\mu}\left(\frac{\partial P}{\partial z} + \rho g\right) \quad (5)$$

where q_x and q_z are the specific discharges in *x* and *z* directions, respectively [LT^{-1}]; μ is the dynamic viscosity [$ML^{-1}T^{-1}$]; k_x and k_z represent the intrinsic permeabilities [L^2] in the two coordinate directions; g is the gravitational acceleration constant [LT^{-2}].

The governing equation with sink/source terms for variable-density flow in terms of equivalent freshwater head can be derived as follow, with a coordinate system transfer aligned with the principal directions of permeability:

$$\frac{\partial}{\partial \alpha}\left(\rho K_{f\alpha}\left[\frac{\partial h_f}{\partial \alpha} + \frac{\rho - \rho_f}{\rho_f}\frac{\partial Z}{\partial \alpha}\right]\right) + \frac{\partial}{\partial \gamma}\left(\rho K_{f\gamma}\left[\frac{\partial h_f}{\partial \gamma} + \frac{\rho - \rho_f}{\rho_f}\frac{\partial Z}{\partial \gamma}\right]\right) = \rho S_f \frac{\partial h_f}{\partial t} + \theta \frac{\partial \rho}{\partial C}\frac{\partial C}{\partial t} - \bar{\rho} q_s \quad (6)$$

where α represents the principal direction of permeability parallel to the bedding; γ represents the direction normal to the medium bedding; $K_{f\alpha}$ and $K_{f\gamma}$ are the freshwater hydraulic conductivities in the α and γ directions, respectively [LT^{-1}]; S_f is the specific storage in term of the freshwater head [L^{-1}]; C is the solute concentration (salinity) [ML^{-3}]; $\bar{\rho}$ is the density of water entering from a source or leaving through a sink [ML^{-3}]; q_s is the volumetric flow rate per unit volume representing sink/source term [LT^{-1}].

2.2.2 Variable-Density Groundwater Flow in a Conduit

Groundwater flow within a fully saturated karst conduit can be assumed as one-dimensional along the axis of straight cylindrical pipe. The Darcy-Weisbach equation is used to calculate head and specific discharge within the pipe, which is applicable to both laminar and turbulent flows [*Shoemaker et al.*, 2008]:

$$\Delta h = h_L = \lambda \frac{\Delta l}{d}\frac{v^2}{2g} \quad (7)$$

where Δh or h_L is the head loss [L] along the pipe length Δl [L]; λ is the friction factor [dimensionless]; d is the pipe diameter [L]; v is the mean velocity [LT^{-1}]; g is the gravitational acceleration constant [LT^{-2}].

On the other hand, the Bernoulli equation with head loss term between the two end points of a conduit pipe could be written as

$$\frac{p_1}{\rho g} + z_1 + \frac{{v_1}^2}{2g} = \frac{p_2}{\rho g} + z_2 + \frac{{v_2}^2}{2g} + h_L \quad (8)$$

where p_1 and p_2 are the fluid pressures at the two points [MLT^{-2}], z_1 and z_2 are the elevations at the two points [L], v_1 and v_2 are the velocities [ML^{-1}] at the two points, respectively, which are assumed the same at the two ends of a conduit tube, since only the averaged velocity is calculated within a tube; h_L is the head loss [L] of water flow along the two ends of a conduit tube. The head loss term in Bernoulli equation and Darcy-Weisbach equation along the pipe can be reformulated as

$$h_L = \frac{p_1 - p_2}{\rho g} + z_1 - z_2 = \lambda \frac{\Delta l}{d} \frac{v^2}{2g} \quad (9)$$

The mean pipe flow velocity (v) can be calculated by the volumetric flow rate, Q [L^3T^{-1}], divided by the cross-sectional area A [L^2] that is perpendicular to flow direction. The density-dependent Darcy-Weisbach equation is reformulated to solve for volumetric flow rates in term of head loss as

$$Q = A \cdot v = A\sqrt{\frac{\Delta h \ d \ 2g}{\Delta l \ \lambda}} = A\sqrt{\frac{2gd}{\lambda \Delta l}\left(\frac{p_1 - p_2}{\rho g} + z_1 - z_2\right)} = A\sqrt{\frac{2gd}{\lambda}\left(-\frac{1}{\rho g}\frac{dp}{dl} - \frac{dz}{dl}\right)} \quad (10)$$

The relationship of pressure and equivalent freshwater head [*Guo and Langevin*, 2002] is used to derive the equation of variable-density groundwater flow in the conduit,

$$p = \rho_f g (h_f - z) \quad (11)$$

The equation of flow rate respect to equivalent freshwater head and density could be represented by substituting the pressure term in equation 10 as

$$Q = A\sqrt{\frac{2gd}{\lambda}\left(\frac{\rho_f g}{\rho g}\frac{dh_f}{dl} - \frac{\rho_f g}{\rho g}\frac{dz}{dl} + \frac{dz}{dl}\right)} = A\sqrt{\frac{2gd}{\lambda}\left(\frac{\rho_f}{\rho}\frac{dh_f}{dl} + \frac{\rho - \rho_f}{\rho}\frac{dz}{dl}\right)} \quad (12)$$

Hybrid models are widely used to study groundwater flow and solute transport in a karst aquifer. Nonlaminar conduit flow is coupled with Darcian flow in a porous medium with an exchange between the two domains. Groundwater flow exchange through the pipe wall between the conduit and the surrounding porous medium is calculated by a linear relationship model [*Shoemaker et al.*, 2008]

$$Q_{n,ex} = \alpha_n \left(h_{f,n} - h_{f,\ i,k}\right) \quad (13)$$

where $Q_{n,ex}$ is the volumetric exchange flow rate between the conduit and matrix [L^3T^{-1}]; h_n is the equivalent freshwater head at conduit node *n* [L] calculated from equation 12; $h_{i,k}$ is the equivalent freshwater head at matrix cell *i, k* [L] calculated from equation 13; the pipe conductance α_n at conduit node *n* [L^2T^{-1}] is calculated by

$$\alpha_n = \frac{\sum_t^2 K_l^t \pi d_l^t \frac{1}{2}\left(\Delta l_l^t \tau_l^t\right)}{r_l^t} \quad (14)$$

where the superscript *t* indicates either forward or backward direction of the pipe connected to node *n*; K_l^t is the conduit wall permeability term for pipe *l* [LT^{-1}]; π is the mathematical constant pi [dimensionless]; $d_l^\dagger$ is the diameter of pipe *l* [L]; $\Delta l_l^\dagger$ is the straight-line length of pipe *l*[L]; $\tau_l^\dagger$ is the tortuosity of pipe *l* [dimensionless]; $r_l^\dagger$ is the radius of pipe *l* [L].

2.3 Transport Modeling

The advection-dispersion equation is widely used in the numerical transport models, such as MT3DMS [*Zheng and Wang*, 1999; *Zheng and Bennett*, 2002] and UMT3D [*Spiessl et al*., 2007]. The second-order partial differential equation is simplified as two-dimensional in this study as,

$$\frac{\partial(\theta C)}{\partial t} = \frac{\partial}{\partial x_i}\left(\theta D_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(\theta v_i C) + q_s C_s \quad (15)$$

where θ is the effective porosity of the porous medium [dimensionless]; v_i is the seepage or linear pore water velocity [LT^{-1}], which is related to the specific discharge or Darcian flux through the relationship, $v_i = q_i/\theta$; C is the solute concentration [ML^{-3}]; D_{ij} is the hydrodynamic dispersion coefficient tensor [L^{2}T^{-1}]; C_s is the solute concentration of water entering from sources or flowing out from sinks [ML^{-3}]; q_s is volumetric flow rate per unit volume of aquifer representing fluid source (positive) and sink (negative) [T^{-1}], including the solute exchange with the conduit node in equation 17.

In this study, conduit solute transport within the tube is describe by the one-dimensional advection-dispersion equation,

$$\frac{\partial C_l}{\partial t} = -v\frac{\partial C_l}{\partial x} + D_{dis}\frac{\partial^2 C_l}{\partial x^2} \quad (16)$$

where C_l is the solute concentration in the conduit tube *l* [ML^{-3}]; v is the conduit flow velocity in the conduit tube *l* [LT^{-1}], which can be calculated by volumetric flow rate Q from the Darcy-Weisbach equation [L^{3}T^{-1}]; D_{dis} is the dispersion coefficient within the conduit. Note that there are no sink/source terms in the advection-dispersion transport equation within the conduit, because the sink/source terms and exchanges with the surrounding porous media are computed at the conduit nodes only.

The solute advective exchange rate between a conduit node and the surrounding porous medium cell is determined by

$$K_{ex,n} = \begin{cases} \dfrac{Q_{n,ex}^{+} C_{i,k}}{V_{i,k}}, & Q_{n,ex}^{+} > 0 \\ \dfrac{Q_{n,ex}^{+} C_{n}}{V_{i,k}}, & Q_{n,ex}^{+} < 0 \end{cases} \quad (17)$$

where $K_{ex,n}$ is the solute advective exchange rate between a conduit node *n* and respective matrix cell *i*, *k* [ML^{-3} T^{-1}]; $Q_{n,ex}^{+}$ is the exchange flow rate [L^{3}T^{-1}] at the conduit node *n calculated from equation* 13 (where $Q_{n,ex}^{+} > 0$, flow direction is from the matrix to the conduit node; where $Q_{n,ex}^{+} < 0$, flow direction is from the conduit node to the matrix); $C_{i,k}$ is the solute concentration at cell *i, k* in the porous medium at conduit node *n* [ML^{-3}]; C_n is the nodal concentration at conduit node *n* [ML^{-3}]; $V_{i,k}$ is the volume of cell *i, k* of the porous medium at conduit node *n* [L^3]. *Spiessl et al*. [2007] pointed out that mass transport within a conduit networks is determined by the flow velocity within the conduits, the exchange coefficients between the conduit nodes and porous matrix, the magnitude of conduit sink/source terms and the lengths of conduit tubes. Mathematically, a weighted arithmetic mean of the nodal concentration value C_n [ML^{-3}] at conduit node *n* can be expressed as follow [*Spiessl et al*., 2007]:

$$C_n = \frac{\sum_t^2 Q_{n,l}^{t+} C_{n,l}^{t} + Q_{n,ex}^{+} C_{i,k} + \sum_s Q_{n,s}^{+} C_{n,s}}{\sum_t^2 Q_{n,l}^{t+} + Q_{n,ex}^{+} + \sum_s Q_{n,s}^{+}} \quad (18)$$

where superscript *t* indicates either forward or backward direction of the pipe connected to node *n*; $C_{n,l}^{t}$ is the concentration of tube *l* connected to face *t* of the conduit node *n* [ML^{-3}]; $C_{n,s}$ is the concentration of the source or sink term to the conduit node *n* [ML^{-3}]. The superscript +represents the inflow terms at conduit node *n*, which means that only inflow terms are used to compute the nodal concentration; $Q_{n,l}^{t+}$ is the flow exchange of tube *l* connected to face *t* at the conduit node *n* [L^3T^{-1}]; $Q_{n,s}^{+}$ is the volumetric flow rate of a source term at conduit node *n*[L^3T^{-1}].

2.4 Numerical Implementation and Code Structure

The VDFST-CFP model is written in Fortran language with several packages for solving groundwater flow and solute transport equations in the conduit and the porous medium, respectively. The finite difference method is applied to solve the two-dimensional variable-density Darcian flow governing equations in the continuum porous medium domain. An oscillation-free solution of upstream weighting scheme is applied to determine the interface concentration between two matrix cells. The solution of a variable-density flow field is coupled with and used for the solute transport simulation. The two-dimensional advection-dispersion solute transport equation in the porous medium is numerically solved by the finite difference method as well. Fortran LAPACK (Linear Algebra PACKage) routines are used to solve the linear algebra matrix by implicit finite difference method with backward-difference in time. In the VDFST-CFP model, the numerical approaches for calculating flow and transport within porous media are very similar to MODFLOW [*Harbaugh*, 2005] and the finite difference solvers in MT3DMS [*Zheng and Wang*, 1999]. The variable-density term of the porous medium governing equation in the VDFST-CFP model is the same as that in SEAWAT model [*Guo and Langevin*, 2002].

In the Darcy-Weisbach equation, the volumetric flow rate within the conduit under turbulent flow condition is nonlinear in respect to the gradient of equivalent freshwater head. In the

VDFST-CFP, Newton-Raphson method is applied to calculate the equivalent freshwater head by forming the Jacobian matrix to solve the system of linear equations iteratively. Nodal heads from the previous time step are used to start Newton-Raphson iterations for the current time step. Specifically, nodal heads are set equal to the head in the porous medium at the beginning of the first time step as initial condition. The numerical approaches for groundwater flow within conduit network is similar to MODFLOW-CFP [*Shoemaker et al*., 2008], except the estimation of the friction factors. The hybrid coupling processes of flow and transport exchange between the conduit and the porous medium are similar to the numerical approach in the discrete-continuum CFPv2/UMT3D model [*Spiessl et al*., 2007; *Reimann et al*., 2014; *Xu et al*., 2015a].

In this study, the friction factors within tubes are updated by the Blasius equation in each iteration of conduit flow calculation, with correlation for curved or helically coiled tubes, and taking into account the equivalent curve radius:

$$\lambda = 0.316 Re^{-\frac{1}{4}} + 0.0075\sqrt{\frac{d}{2R_c}} \quad (19)$$

$$R_c = r\left[1 + \left(\frac{H}{2\pi r}\right)^2\right] \quad (20)$$

where λ is the friction factor [dimensionless], H is the helicoidal pitch [L], and r is the conduit diameter [L].

The implicit finite difference method with backward-difference in time is applied to solve the one-dimensional advection-dispersion equation for salt transport within the conduit. Explicit scheme is used more often for advection problem with less computational cost. However, the numerical stability criterion of the explicit method for solving the advection equation requires that the Courant number (N_{co}) is a small number, generally smaller or equal to 1,

$$N_{co} = \left|\frac{v\Delta t}{\Delta l}\right| \leq 1 \quad (21)$$

where v is the average velocity in the conduit [LT^{-1}]; Δt is the length of timestep [T]; Δl is the length of conduit tube [L].

A small Courant number requires a small time step, since the conduit flow can be several orders of magnitudes faster than Darcian flow and usually turbulent. As a result, the implicit scheme is used instead of explicit scheme, because of its advantage of unconditionally numerical stability. Other explicit semi-Lagrangian schemes, such as the EMCNOT by *Liu et al*. [2001], are applied in CFPv2/UMT3D model for solute transport within conduit [*Spiessl*, 2004; *Spiessl et al*., 2007], but not in this study because of the coding complexity and additional computational cost. In the

VDFST-CFP model, each tube is subdivided into 10 segments with higher spatial resolution in order to reduce numerical dispersion error in conduit transport simulation.

Implicit approach is used to solve groundwater flow and solute transport equations in an iterative sequence in each time step, until the consecutive differences of the calculated head and density are less than the specified convergence values. In the implicit iterations of flow and transport coupling, the acceptable maximum density and head differences in a matrix cell and conduit node are set as very small values, especially in the highly permeable conduit network. In the beginning of an implicit iteration loop, the variable-density flow equations for the porous medium and the conduit are solved by the finite difference method and Newton-Raphson method, respectively. After that, the two-dimensional advection-dispersion transport equations in the porous medium and the one-dimensional advection-dispersion transport equation in the conduit are solved by the implicit finite difference method. The conduit nodal concentrations are calculated by the weighted arithmetic mean relationship expressed in equation 18. The water budgets of both the conduit and porous medium systems are calculated at the end of each time step. The computational cost and model elapsed time are tremendous in the implicit iterations, because flow and transport equations are iteratively solved multiple times in each time step. However, explicit method is unacceptable in this study due to numerical stability and model convergence requirements.

3 Simulation Results

3.1 Comparison of Models

The simulation results by the VDFST-CFP model are compared with those by other numerical models, such as SEAWAT [*Guo and Langevin*, 2002], in which a variable-density groundwater flow model is coupled with a solute transport model, such as MODFLOW/MT3DMS [*Zheng and Wang*, 1999; *Harbaugh*, 2005] and CFPv2/UMT3D [*Spiessl et al*., 2007; *Reimann et al*., 2013] models, which are constant density continuum model and hybrid discrete-continuum model, respectively.

In the constant density MODFLOW/MT3DMS and CFPv2/UMT3D models, the equivalent freshwater heads are precomputed and substituted in the constant head boundary conditions. On the other hand, the equivalent freshwater heads are directly calculated in the density-dependent SEAWAT and the VDFST-CFP models without any preprocessing. In the SEAWAT, MODFLOW/MT3DMS, and CFPv2/UMT3D models, the PCG solver in MODFLOW numerically solves the flow equations, and the GCG solver in MT3DMS numerically solves the solute transport equations. The numerical methods in the newly developed VDFST-CFP model are very similar to other numerical models. In the hybrid model, laminar groundwater flow in the carbonate rock matrix is simulated by a two-dimensional, single continuum porous medium equivalent model using the Darcy equation, and linked to a one-dimensional pipe flow model that simulates laminar or nonlaminar flow in the conduits using the Darcy-Weisbach equation. Water and solute exchange between the two domains is calculated via a head-dependent flux boundary condition and solved iteratively until the head solutions converge.

For comparison purpose, the values of hydrological parameters in the conduit and the porous medium are identical in different models, including the hydraulic conductivity, specific storage, effective porosity, and dispersivity. The conduit is represented as continuum grid cells with large hydraulic conductivity, specific storage, and effective porosity in MODFLOW and SEAWAT models, in which groundwater flow is still simulated by the Darcy equation. Effective porosity and specific storage of the conduit network represented by porous medium cells in the continuum model are simply calculated by the percentage of void space volume. The calculation of hydraulic conductivity in the conduit can be tricky in the VDFST-CFP model. The following approach is used to calculate the conduit diameters and friction factors in the discrete-continuum models, to be equivalent to hydraulic conductivity of the conduit network in the continuum models. First, the transition between laminar and turbulent flow is governed by the Reynolds number,

$$Re=\frac{qd}{v} \quad (22)$$

where Re is the Reynolds number [dimensionless]; q is the specific discharge [LT^{-1}]; defined as discharge per unit cross-section flow area; d is the specific length dimension [L], usually the mean void diameter of porous media or conduit diameter for discrete elements; v is the kinematic viscosity of the fluid [L^2T^{-1}].

In the discrete-continuum model, laminar flow in a cylindrical conduit is described by the linear Hagen-Poiseuille equation 24 below, which is obtained from the Darcy-Weisbach equation if $\lambda=64/Re$, where λ is the friction factor [dimensionless] [*Reimann et al*., 2011b]

$$\frac{\partial h}{\partial x}=-\lambda\frac{q^2}{2gd} \quad (23)$$

$$q=-\frac{gd^2}{32v}\frac{\partial h}{\partial x} \quad (24)$$

On the other hand, the discharge of laminar flow is linearly proportional to the hydraulic gradient and the hydraulic conductivity in the Darcy equation. Specific discharge of conduit flow is calculated by the Darcy equation under laminar condition in the continuum model as follow [*Harbaugh et al*., 2000]:

$$q = -K\frac{\partial h}{\partial x}\quad(25)$$

Therefore, the relationship between conduit hydraulic conductivity in the continuum model and conduit diameter in the discrete-continuum model can be derived from the previous two equations as,

$$K = \frac{gd^2}{32v}\quad(26)$$

However, the estimation of equivalent conduit hydraulic conductivity and conduit diameter is based on laminar flow condition, in which the Reynolds number is smaller than the critical Reynolds number, usually around 2000–4000 [*Reimann et al*., 2011b; *Bear*, 2013]. The uncertainty of this approximation on nonlaminar flow condition will be discussed in section 4.

3.2 Benchmark Cases

Two benchmark cases are setup to test the VDFST-CFP model, one case is a horizontal plane and the other case is a vertical cross section. The horizontal case compares the simulation results of the hybrid discrete-continuum models and continuum models. On the other hand, the vertical case tests the performance of density-dependent flow and transport simulation. The numerical models are set identical with the same grid discretization, boundary conditions, and equivalent parameter values in each benchmark.

The conceptual model, grid discretization and boundary conditions of the two-dimensional horizontal case are shown in Figure 1. The finite difference spatial domain discretization consists of 21 rows, 120 columns, and 1 layer. The row and column dimensions for each cell are 500 ft by 500 ft, with 50 ft thickness in the horizontal plane. The conduit network is located along row #11 in the middle of the spatial domain from left to right. The conduit is discretized into 119 tubes with 120 nodes as well, which are located in the center of the surrounding porous medium cells. As mentioned in section 2.4, each tube is subdiscretized into 10 segments in the solute transport simulation. The elevation of the horizontal plane is set in a deep confined aquifer layer, which starts from 334 ft BSL (below sea level) on the left (seawater boundary) and gradually rises to 319 ft BSL on the right (freshwater boundary). The horizontal case is designed to simulate seawater intrusion through deep karst conduits, which are commonly observed in many coastal karst aquifers, for example, the Floridan aquifer in the Woodville Karst Plain, Florida [*Werner*, 2001; *Loper et al*., 2005; *Kernagis et al*., 2008; *Kincaid and Werner*, 2008; *Xu et* *al*., 2016]. In the MODFLOW and SEAWAT continuum model, the HFB (Horizontal-Flow Barrier) package is used to set the exchange permeability between conduit and porous medium.

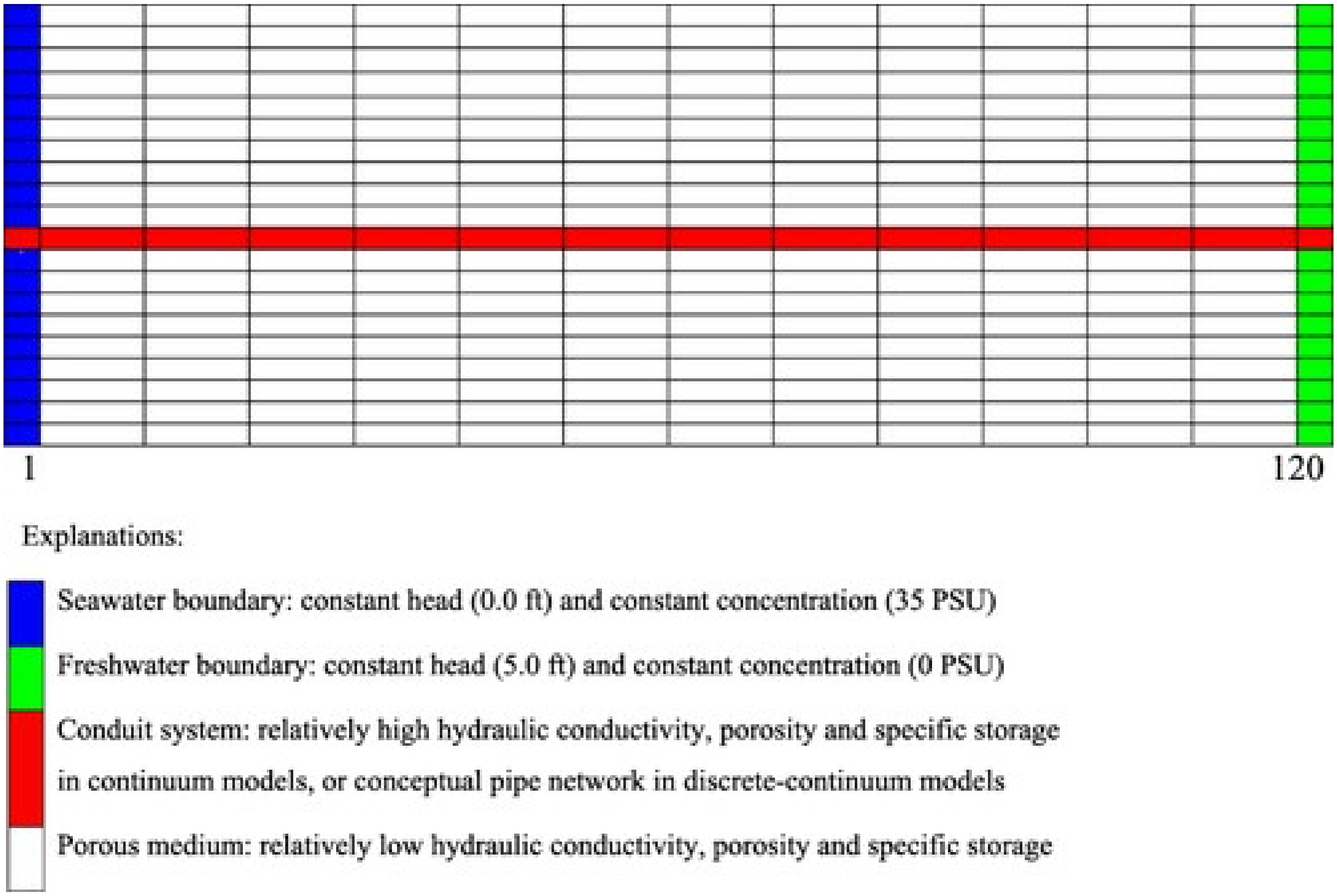

Figure 1

Open in figure viewerPowerPoint

Schematic figure of finite difference grid discretization and boundary conditions applied in the horizontal benchmark cases. Every horizontal cell shown represents 10 cells, except the two boundaries, represents smaller widths. The conduit system is located at row #11 in the middle of the domain, which starts from column #1 on the left to #120 on the right.

Caption

In the horizontal benchmark, the freshwater boundary on the right is assigned as constant head (5.0 ft) and constant concentration (0.0 PSU) to represent regional freshwater recharge. The saline water boundary on the left is assigned as constant head (0.0 ft) and constant concentration (35.0 PSU) to represent hydrostatic condition of seawater. The head boundary on the left of the conduit is set as constant 1.0 ft, higher than the head in the surrounding porous media in order to accelerate the exchanges between conduit and surrounding porous media. The head boundary on the right of the conduit remains 5.0 ft to be the same as that in the porous media. In the constant-density numerical models, the head boundary on the seawater side is substituted by the precomputed equivalent freshwater head by salinity, density, and elevation using equations 2 and 3. The upper and lower boundaries are no-flow boundaries.

In the continuum SEAWAT and MODFLOW/MT3DMS models in the horizontal case, 100 time steps are required to run a 1 day simulation with the specified length of time step as 0.01 days. However, 1000 time steps are needed in the discrete-continuum models, such as CFPv2/UMT3D and the VDFST-CFP, with smaller time step size specified as 0.001 days. The convergence criteria are more rigorous for the discrete-continuum numerical models, which is discussed in section 4. The total CPU time of the VDFST-CFP model in the horizontal case is about 925 min on a 2.9 GHz Intel Core i7 processor.

In the two-dimensional vertical benchmark case, variable-density SEAWAT and the VDFST-CFP model are compared. Constant density models such as MODFLOW and CFPv2/UMT3D are not applicable in the vertical benchmark case, because the vertical flux simulations without variable-density modeling are physically inappropriate and the simulation results are not reasonable. In Figure 2, the spatial domain discretization consists of 1 row, 140 columns, and 37 layers in the vertical cross section. The row and column dimensions of each cell are 50 ft by 50 ft with 10 ft thickness in each layer. The conduit system starts from the top of column #22, descends downward to layer #29, horizontally extends from column #22 to column #139, finally rises upward to the surface through column #139. Similar to the horizontal benchmark, the conduit network is discretized into 173 tubes with 174 conduit nodes in the center of each grid cell. The top layer elevation starts from 34 ft BSL (below sea level) on the left and gradually rises to 19 ft BSL on the right. The vertical benchmark simulates a confined aquifer with an impermeable surface on the top.

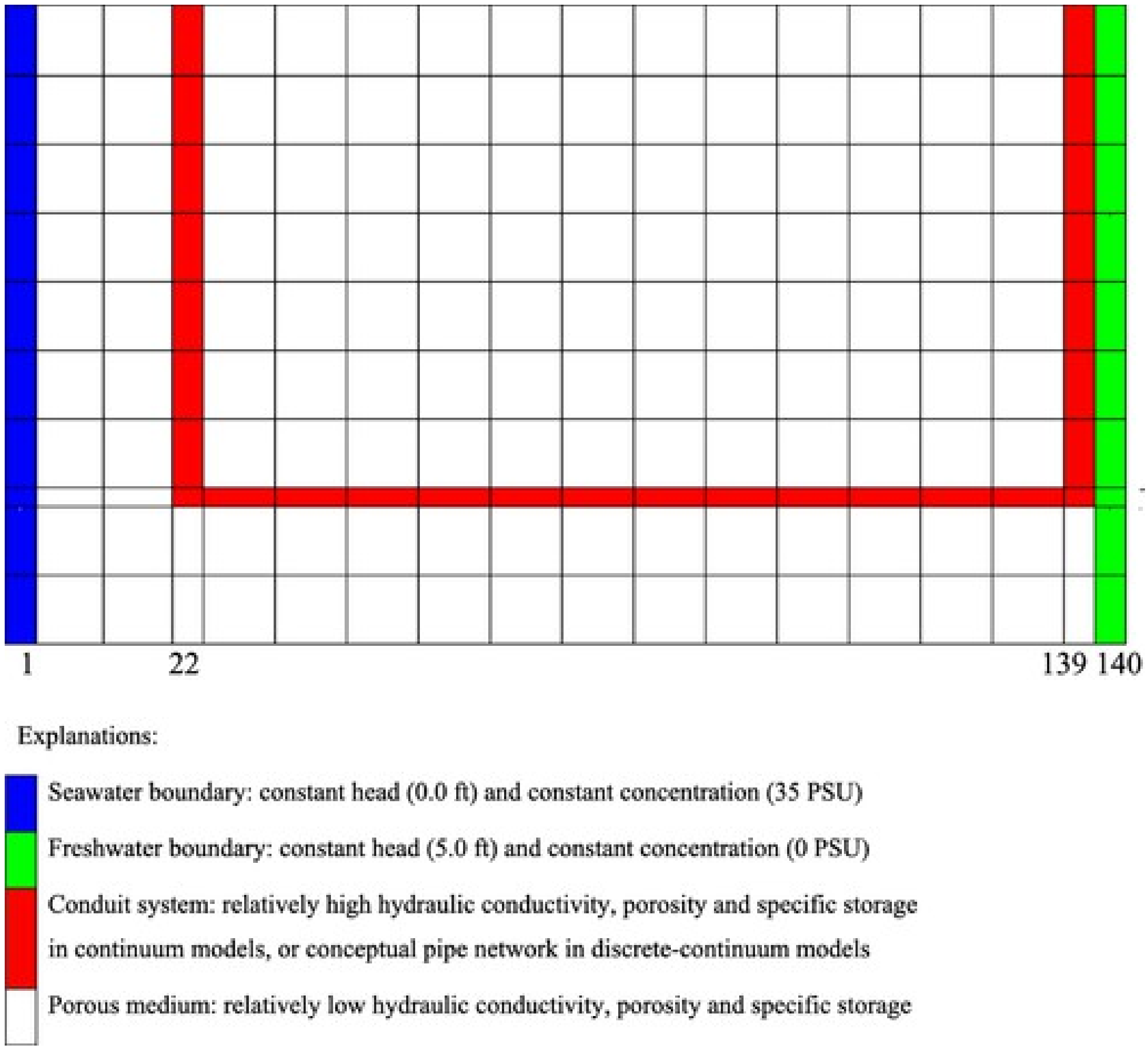

Figure 2

Open in figure viewerPowerPoint

Schematic figure of finite difference grid discretization and boundary conditions applied in the vertical benchmark case. Each cell represents 10 horizontal cells and 4 vertical cells, except the two boundaries and the conduit layer, which are shown with smaller dimensions. The conduit system starts from the top of column #22, descends downward to layer #29, horizontally extends to from column #22 to column #139, and then rises upward to the top through column #139.

Caption

The boundary conditions of the porous medium in the vertical case are very similar to those in the horizontal case, in which the constant head and concentration boundary of freshwater (5.0 ft, 0.0 PSU) and seawater (0.0 ft, 35.0 PSU) are on the right and left sides, respectively. The initial conditions of the conduit system are the same as surrounding porous medium. The top and bottom are no-flow boundaries. In the continuum SEAWAT model, there are 40 time steps in the 0.2 day simulation period with the time step size as 0.005 day. However, the VDFST-CFP model needs 400 time steps to run the same simulation period with smaller time step size as 0.0005 day, due to the more rigorous convergence criteria in the discrete-continuum numerical model. The total CPU time required by the VDFST-CFP model in the vertical case is approximately 1350 min.

The definitions and values of hydrological parameters in the porous medium and the conduit are listed in Table 1. The values of porous medium parameters in the two benchmarks are assigned by the hydrogeological properties of the Upper Floridan Aquifer (UFA) in the WKP. The parameters were calibrated in a regional-scale numerical model by *Davis et al*. [2010] and then applied in many subsequent modeling studies [*Gallegos et al*., 2013; *Xu et al*., 2015a, 2015b]. However, the values of diameter and friction factor of the conduit network are synthetic and do not match with field conditions, because of the limitations of discrete-continuum modeling method to the applications of variable-density flow and transport simulations, which are discussed in section 4. The exchange permeability is assumed constant, and same as the hydraulic conductivity value in the porous medium.

Table 1. Parameters Values in Porous Medium and Conduit in the Horizontal and Vertical Casesa

	Porous Media	**Conduit (Continuum Model)**	**Conduit (Discrete Model), Horizontal Benchmark**	**Conduit (Discrete Model) Vertical Benchmark**
Conductivity (ft/day)	7500	2×10^{6}		
Effective porosity	0.003	0.031		
Specific storage	5.0×10^{-5}	1.0×10^{-4}		

	Porous Media	Conduit (Continuum Model)	Conduit (Discrete Model), Horizontal Benchmark	Conduit (Discrete Model) Vertical Benchmark
Dispersivity (ft)	32.80	0		
Diameter (ft)			3.00	0.891/1.333b
Friction factor			0.0178	0.03

- a MODFLOW/MT3DMS and SEAWAT are continuum models, while MODFLOW-CFP/UMT3D and the VDFST-CFP are discrete-continuum models. Conduit parameters including diameters and friction factors are different in horizontal and vertical benchmarks.
- b In the vertical case, the conduit diameter of horizontal part is calculated as 0.891 ft, but is calculated as 1.333 ft in the vertical parts of the conduit.

3.3 Model Validation

The VDFST-CFP model validation is tricky and not easy, because the analytical solution of such complicated hybrid model is very difficult or even impossible to derive. On the other hand, very few studies have reported field observation and continuous measurement of seawater intrusion through a subsurface coastal karst conduit system. Currently, the VDFST-CFP model is not yet able to simulate seawater intrusion through giant conduit networks with large diameters in the field. The other possible model validation approach is to turn off the discrete conduit network in the VDFST-CFP, use exactly the same parameters for the conduit as the continuum SEAWAT model, and compare the results with other models. However, this approach is inappropriate neither, because conduit flow rate is a nonlinear function of head gradient, and groundwater flow through conduit networks cannot be accurately simulated by the Darcy equation. The application of finite difference method for conduit transport simulation with rapid flow velocity is an issue that needed to be studied in the future.

In this section, the head simulation results by CFPv2 model are used to compare and validate the VDFST-CFP model in both conduit network and porous medium (Figure 3). It is appropriate to compare the results between these two discrete-continuum models instead of the continuum models with different methods. The results are expected to be similar but not going to be identical, because the friction factor equations are slightly different in the two models.

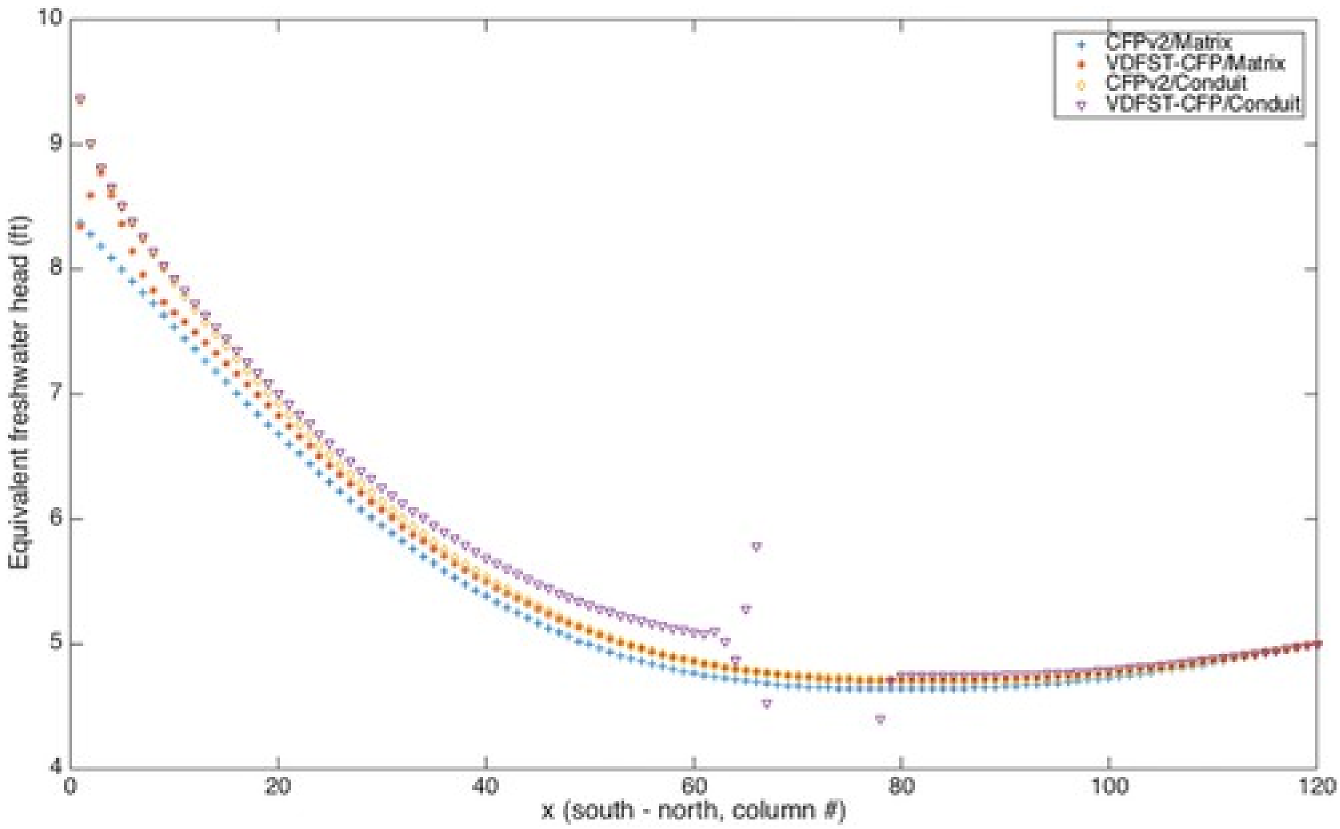

Figure 3

Open in figure viewerPowerPoint

Simulated equivalent freshwater head in conduit network and porous medium: comparison between the VDFST-CFP and CFPv2.

Caption

The equivalent freshwater head is 9.375 ft on the left side of the conduit network, and then decreases to 5.0 on the right freshwater boundary. Head simulation in the conduit are very similar for the two models, in which more than 95% results are within the margin of error at 95% confidence interval. In the VDFST-CFP model, the head instability error is found between columns #60-80 within the conduit, the interface of seawater and freshwater. The instability of head in the conduit is probably due to the instantaneous feedback from the truncation error of solute transport by the finite difference method with a rapid conduit flow, since flow and transport equations are coupled and solved iteratively. On the other hand, the equivalent freshwater head at row #9 or #13 in the porous medium decreases from 8.735 ft on the seawater boundary to 5.0 ft on the right. The head simulations in the porous medium are similar to each other as well by the two models, in which all results are within the margin of error at 95% confidence interval. The simulated equivalent freshwater head is slightly higher in both the conduit network and porous medium by the VDFST-CFP, but the exchanges between the two domains calculated by the two methods are roughly similar to each other. Generally speaking, the VDFST-CFP model is well validated by comparing the results of head simulation in CFPv2 model.

3.4 Simulation Results

Head simulation results by SEAWAT, MODFLOW/MT3DMS, CFPv2/UMT3D, and the newly developed VDFST-CFP numerical models are presented in Figure 4. Simulation results of equivalent freshwater heads in the four models are almost identical. Head results are presented in the figures below instead of equivalent freshwater head, which decreases uniformly from the right to the left boundary, and does not show density effects. The head profile follows the shape of salinity plume and presents the solute transport result as well. The flow field simulations by SEAWAT and MODFLOW continuum models are almost the same, and head profiles of the discrete-continuum CFPv2 and VDFST-CFP models are similar to each other as well. The correlation coefficients of head simulation results are 0.707 in the conduit and 0.624 in the porous medium between two hybrid models VDFST-CFP and CFPv2/UMT3D. The correlation coefficients of head simulation results between the two density-dependent models VDFST-CFP and SEAWAT are 0.916 in the conduit and 0.640 in the porous medium.

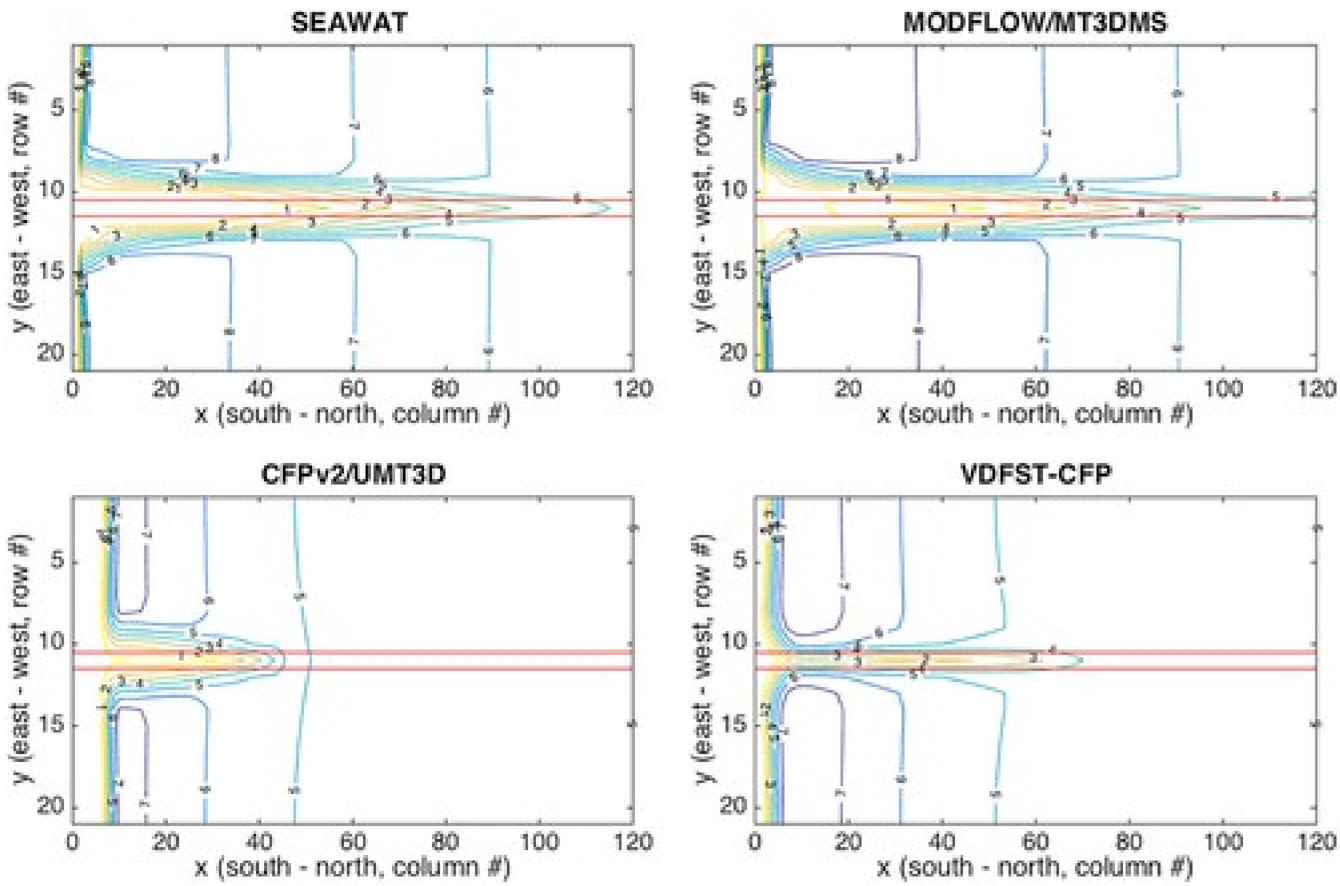

Figure 4

Open in figure viewerPowerPoint

Head simulation results by the two continuum numerical models and the other two discrete-continuum numerical models in the horizontal benchmark: (top left: 1) SEAWAT; top right: 2) MODFLOW/MT3DMS; (bottom left: 3) CFPv2/UMT3D; and (bottom right: 4) VDFST-CFP.

Caption

Apparently, the differences of the solute transport simulation results originate from the different flow fields in the four models. The simulated salinity profiles in the horizontal benchmark by the four models are presented in Figure 5. Generally speaking, seawater intrudes rapidly and significantly along the high-permeability conduit system from left to right, and also flows into the surrounding matrix domain through the exchange between the conduit and the porous medium. Simulation results of continuum models, SEAWAT and MODFLOW/MT3DMS, are exactly the same. The results of discrete-continuum models, CFPv2/UMT3D and the VDFST-CFP, are similar to each other as well. Simulation results of both constant density and variable-density models are supposed to be similar, because the equivalent freshwater heads are precalculated at the seawater boundary, and vertical flux is not simulated in the horizontal benchmark. The correlation coefficients of the salinity results are 0.685 in the conduit and 0.828

in the porous medium between two hybrid models VDFST-CFP and CFPv2/UMT3D. The correlation coefficients of results between the two density-dependent models VDFST-CFP and SEAWAT are 0.913 in the conduit and 0.670 in the porous medium.

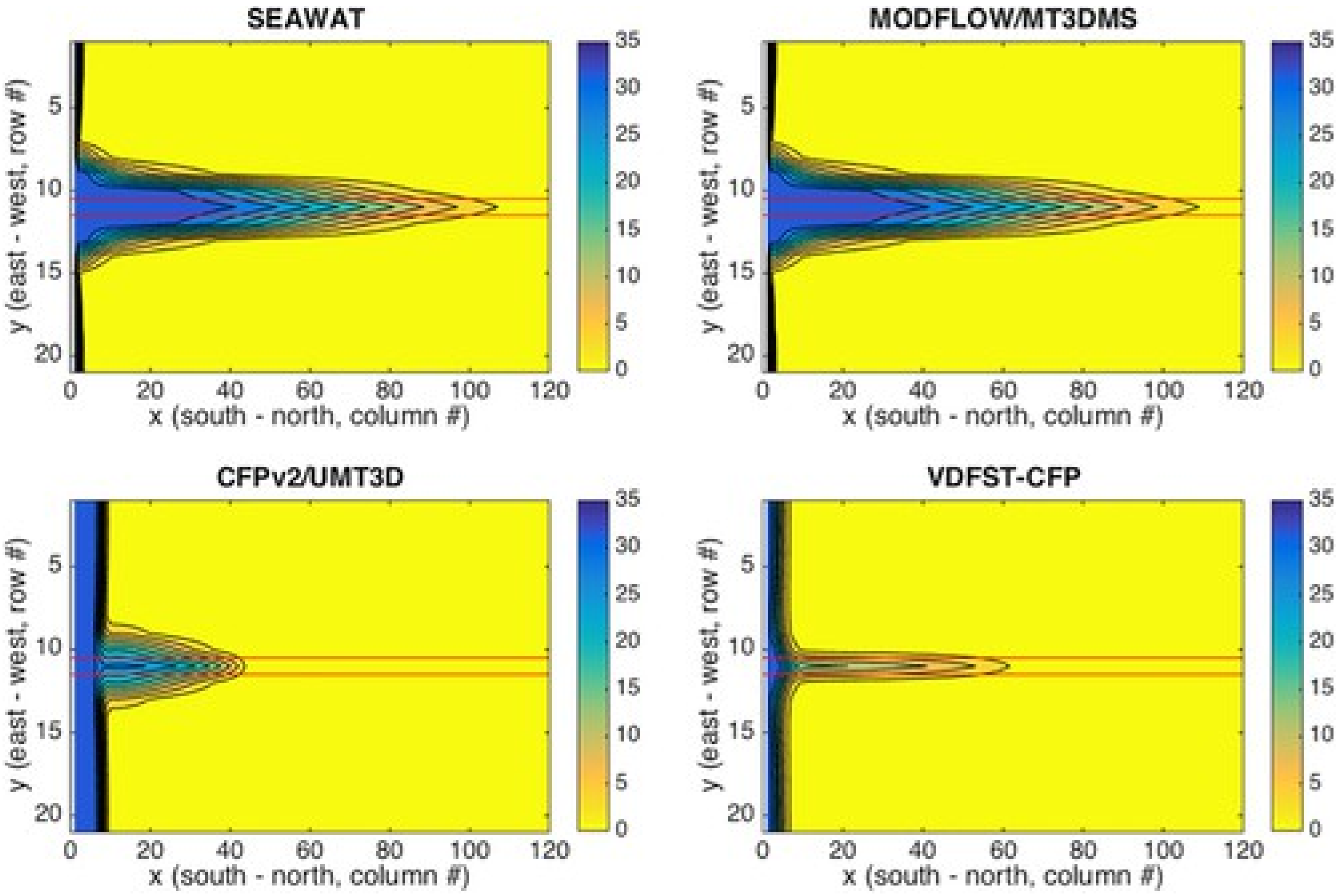

Figure 5

Open in figure viewerPowerPoint

Salinity simulation results by the two continuum numerical models and the other two discrete-continuum numerical models in the horizontal benchmark: (top left: 1) SEAWAT; (top right: 2) MODFLOW/MT3DMS; (bottom left: 3) CFPv2/UMT3D; and (bottom right: 4) VDFST-CFP.

Caption

The simulation results of continuum models, SEAWAT and MODFLOW/MT3DMS, show significant further seawater intrusion along the conduit than those in the discrete-continuum CFPv2/UMT3D and the VDFST-CFP models. The distance of seawater intrusion within the conduit in the VDFST-CFP model is further than the result in CFPv2/UMT3D, but less extended than the results in SEAWAT and MODFLOW/MT3DMS. In the horizontal benchmark, volumetric flow rate of rapid conduit flow is no longer linear to the head gradient under nonlaminar condition. In such cases, the linear Darcy equation 23 applied in the continuum models significantly overestimates the volumetric flow rate in the conduit, results in faster flow velocity and further seawater intrusion along the conduit network in SEAWAT and MODFLOW/MT3DMS models. On the other hand, volumetric flow rate in the conduit is not overestimated by the Darcy-Weisbach equation in CFPv2 and the VDFST-CFP model, considered as an advantage of the hybrid discrete-continuum model used for a karst aquifer.

In the vertical benchmark, head simulation results by SEAWAT and the VDFST-CFP models are presented in Figure 6. Again, head is presented instead of equivalent freshwater head with a better description of flow field and solute transport in the vertical benchmark. The head profile increases from 0 ft from the seawater boundary on the left to 5 ft at freshwater boundary on the right. The correlation coefficients of head results between the two models are 0.912 in the conduit and 0.955 in the porous medium. Flow solutions of the two models are similar, driving solute transport in the conduit network and porous medium.

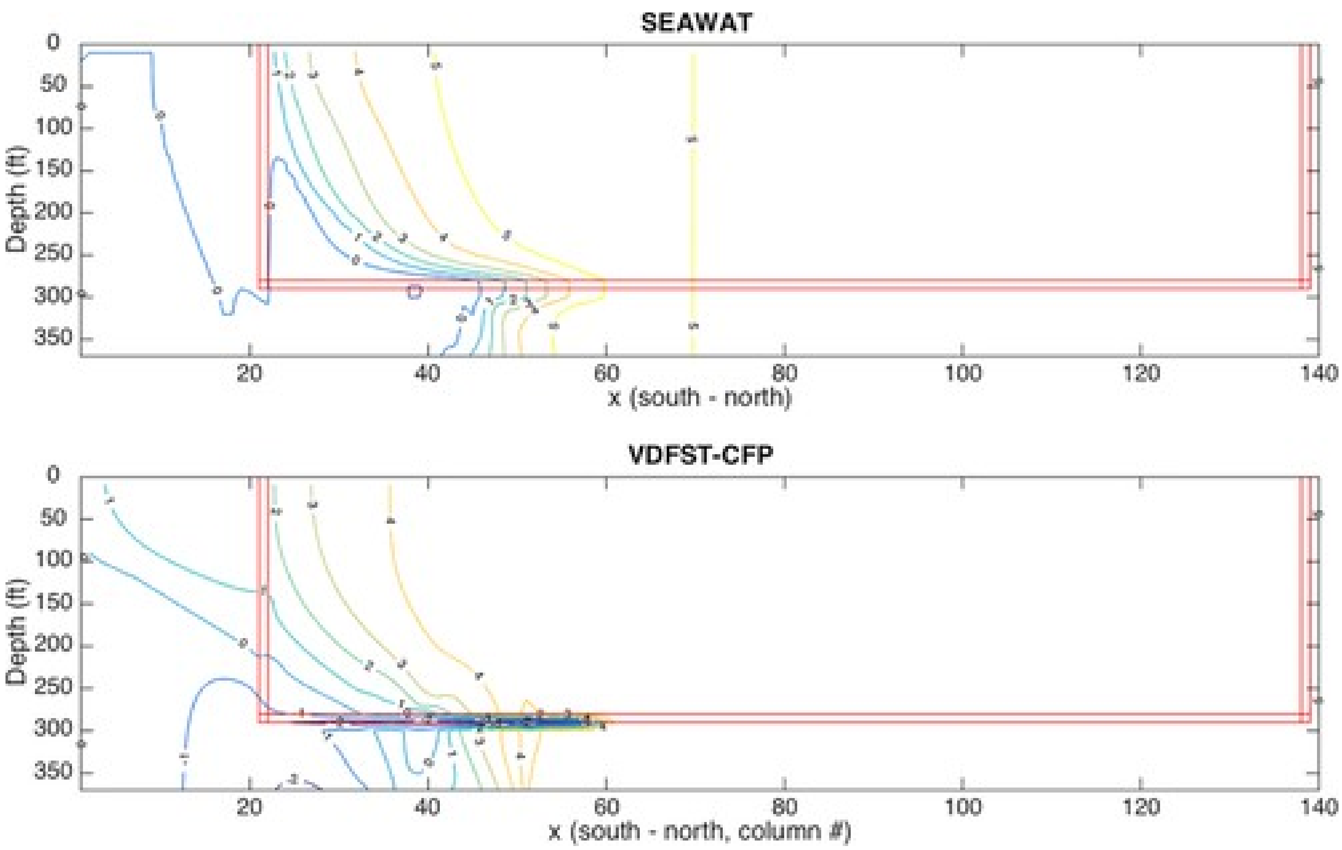

Figure 6
Open in figure viewerPowerPoint
Head simulation results by two density-dependent numerical models in the vertical case: (top: 1) SEAWAT; (bottom: 2) VDFST-CFP. Note that the simulated head distribution along the conduit is plot in the VDFST-CFP result.

Caption

The simulated salinity profiles in the vertical benchmark by the two models are presented in Figure 7. In the vertical benchmark, the correlation coefficients of simulated salinity results between the two density-dependent models VDFST-CFP and SEAWAT are 0.903 in the conduit and 0.983 in the porous medium. Seawater intrudes through the constant concentration boundary on the left and the submarine cave of conduit network opening to the sea on the surface. Solute transport simulations in the porous medium are roughly same by the two numerical models. The mixing zone positions in the conduit are roughly the same by the two models as well. The linear Darcy equation in SEAWAT does not overestimate the volumetric flow rate through conduit network, since conduit flow is laminar and relatively slow in the vertical benchmark. The fingering effect along the conduit system in the SEAWAT simulation is probably due to the numerical instability of groundwater flow and solute transport exchanges between the highly permeable conduit system and the surrounding porous medium with small hydraulic conductivity. However, the fingering effect is not observed in the discrete-continuum VDFST-CFP model, because the exchange between the conduit and the porous medium is calculated internally in the grid cells where conduit nodes are located. Overall, the VDFST-CFP modeling results match better with those by the SEAWAT in the vertical benchmark, probably because the discrepancy of mass budget in the horizontal benchmark is relatively large with faster flow and a bigger conduit diameter.

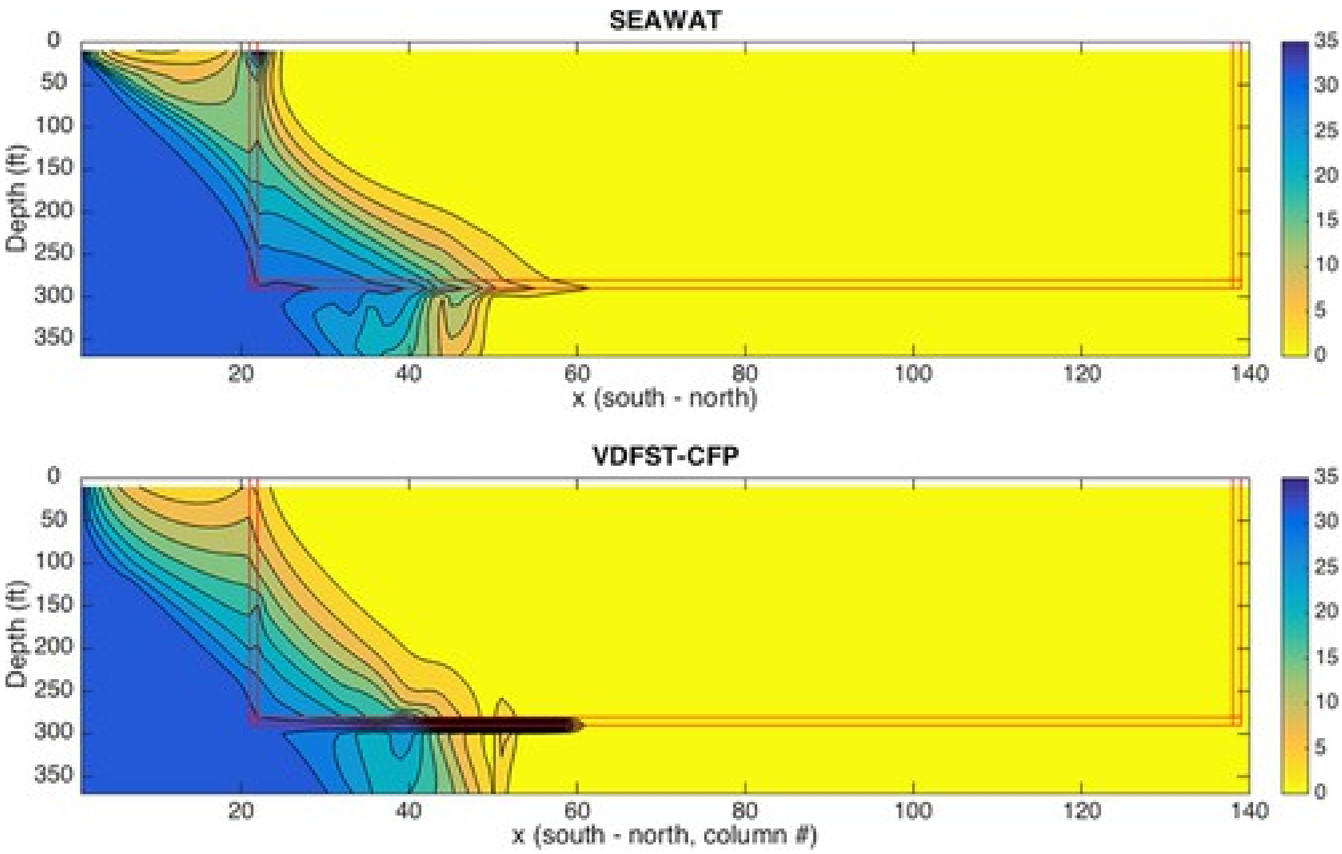

Figure 7

Open in figure viewerPowerPoint

Salinity simulation results by two density-dependent numerical models in the vertical case: (top: 1) SEAWAT; (bottom: 2) VDFST-CFP. Note that the simulated salinity in the conduit is plotted in the VDFST-CFP result.

Caption

3.5 Sensitive Analysis

Sensitivity studies evaluate the importance of several factors for the simulation of seawater intrusion through conduit networks in a karst aquifer. Five parameters in the horizontal benchmark are evaluated in the VDFST-CFP model, including the conduit diameter, friction factor, conduit-matrix exchange interaction, porous medium hydraulic conductivity, and effective porosity. The sensitivity results of exchange permeability, conduit diameter, and friction factor are shown in Figure 8, and the sensitivity results of matrix parameters are shown in Figure 9. The parameter sensitivities in the vertical benchmark are similar to those in the horizontal benchmark and not presented. The positions of the mixing zone, defined as the column numbers of conduit and surrounding porous medium with 10.0 PSU salinity, are evaluated in the sensitivity analysis.

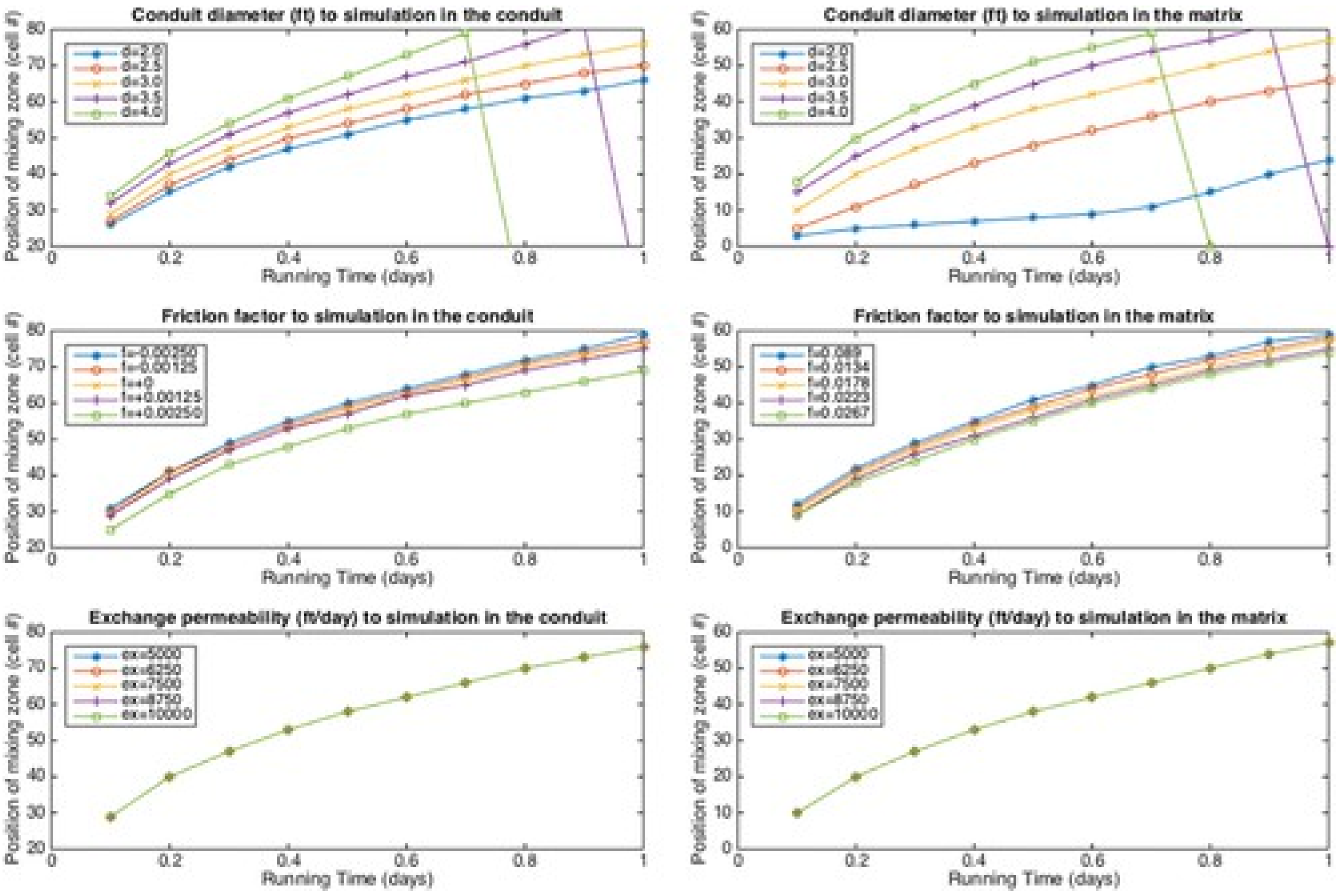

Figure 8

Open in figure viewerPowerPoint

Parameter sensitivity analysis: variation of the position of mixing zone with different conduit parameter values and conduit-matrix interaction. Subplots on the left are simulations in the conduit, and subplots on the right are simulations in porous media. The parameter variations from top to bottom are: (top) d: conduit diameter; (middle) f: friction factor; (bottom) ex: exchange permeability.

Caption

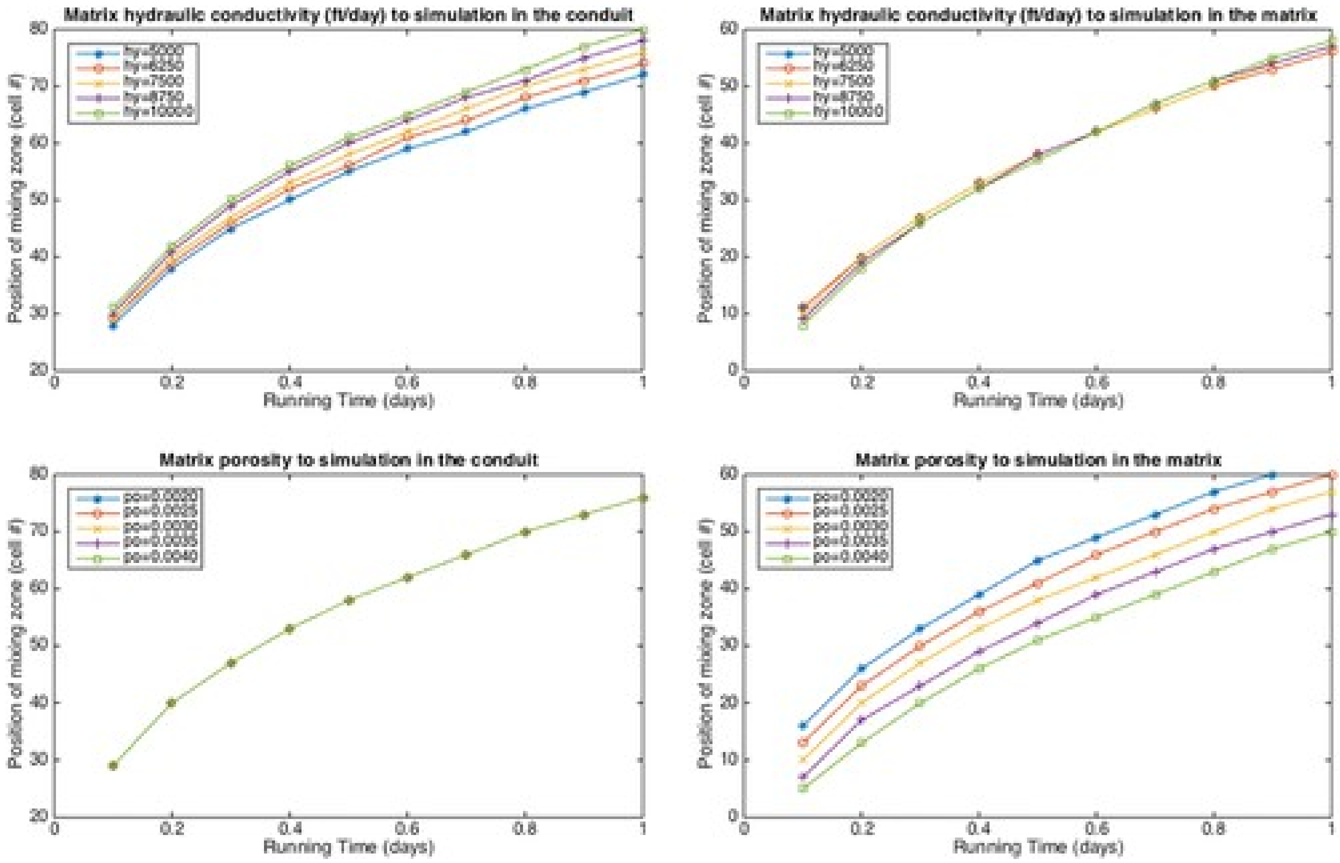

Figure 9

Open in figure viewerPowerPoint

Parameter sensitivity analysis: the mixing zone position due to variation of the of matrix parameters. Subplots on the left are simulations in the conduit, and subplots on the right are simulations in porous media. The parameter variations from top to bottom are: (top) hy: matrix hydraulic conductivity; (bottom) po: effective porosity.

Caption

The conduit diameter is changed from 2.0 to 4.0 ft with an interval of 0.5 ft in the sensitivity study. The mixing zone position moves further landward in the cases with larger diameter, because groundwater flow rate in the large conduit is faster (Figure 8, top). The mixing zone position in the porous medium is affected more significantly with diameter variation, but lags behind the simulation in the conduit. Sensitivity analysis finds out that conduit diameter is an important factor for flow and transport simulation results in both the conduit and porous medium domains. Simulation terminates and model diverges after 0.8 day in the cases with large conduit diameters. The VDFST-CFP model may have serious numerical convergence issue in large conduit diameter cases, due to the limitations and assumptions of discrete-continuum modeling method, which is discussed in section 4.

The sensitivity study of friction factor is made by adding and subtracting an artificial value (0.00250 or 0.00125), as the conduit roughness variation in the Blasius equation 19 (Figure 8, middle). Seawater intrudes further landward through the conduit with a smaller friction factor and faster groundwater velocity in a smoother pipe. The conduit friction factor also greatly affects the position of the mixing zone in the porous medium. However, simulation results do not change as much with variation of friction factor as they do with variation of the conduit diameter.

To investigate the impact of conduit-matrix interaction in the model, simulation results are evaluated with the exchange permeability or pipe wall conductivity adjusted from 5000 to 10000 ft/d, with an interval of 500 ft/d (Figure 8, bottom). The salinity simulation results show that both the conduit and the porous medium are insensitive to the variation of exchange permeability in this case, probably due to the relatively stable flow and solute transport interactions between the two domains. The exchanges through the pipe wall are not significant, since the head difference between the conduit and porous medium is relatively small in the horizontal benchmark. However, the permeability of the pipe wall could be an important parameter in other cases and applications of the VDFST-CFP model, if the conduit-matrix interaction is significant with larger head difference between the two domains.

In the sensitivity study, the hydraulic conductivity of the porous medium is adjusted from 5000 to 10000 ft/d, with an interval of 500 ft/d. For consistency purposes, the exchange permeability of the conduit wall is set equal to the porous medium hydraulic conductivity. The mixing zone position moves further landward in the conduit, but regresses backward in the porous medium with larger values of matrix hydraulic conductivity (Figure 9, top). Accelerated flow velocity in the conduit would result in further seawater intrusion landward, due to faster seepage velocity in the porous medium and stronger water and solute exchanges with conduit. The salinity plume moves extensively in the matrix domain with larger values of hydraulic conductivity, and flows away quickly from the conduit into the surrounding porous medium. However, the mixing zone position in the porous medium is not strongly affected by hydraulic conductivity, since groundwater flows relatively slow in the porous medium.

Effective medium porosity is another important parameter for groundwater flow and solute transport simulation results in the porous medium. The value of effective porosity is changed from 0.02 to 0.04 with an interval of 0.005 in the sensitivity study. The effective medium porosity variation does not significantly affect the seawater movement in the conduit, but greatly impacts the salinity transport in the porous medium (Figure 9, bottom). The salt plume with highly saline water is distributed near the conduit network, because the salt transport and solute exchange between the two systems are relatively slow in the porous medium. Therefore, the mixing zone position in the matrix simulation moves further landward with smaller porosity, due to faster seepage velocity with the same hydraulic conductivity in the porous medium domain.

4 Discussion

The VDFST-CFP model simulates seawater intrusion in a coastal karst aquifer with conduit networks, and compares reasonably well with other models. However, the numerical stability, accuracy, and uncertainty problems of the VDFST-CFP model can be found in the two benchmarks. These issues originate from the concepts of discrete-continuum model, numerical methods, governing equations and convergence criteria. The model uncertainty factors are discussed in details below.

First and most importantly, the conduit diameter is limited to be small in the VDFST-CFP model. The hybrid discrete-continuum numerical model requires that the conduit diameter must be one order of magnitude smaller than the finite difference grid cell size where conduit nodes are located. To keep the water budget balance and ensure numerical stability in the discrete-continuum model, the storage and volume of the conduit system should be negligible, compared to the relatively large grid size of the surrounding medium domain [*Shoemaker et al*., 2008; *Reimann and Hill*, 2009; *Reimann et al*., 2014]. On the other hand, relatively fine vertical discretization is required in the variable-density numerical models for the accuracy of density-dependent vertical flux calculation [*Werner et al*., 2013]. In the variable-density SEAWAT model, *Guo and Langevin* [2002] pointed out that a very high grid resolution in the vertical direction is often required to represent the complex flow pattern with large concentration gradients for density-dependent flow and solute transport simulation. Generally speaking, the layer thickness in vertical discretization is usually smaller than 10 ft for the accuracy of density-dependent vertical flux simulation. Meanwhile, the conduit diameter has to be even significant smaller than the high-resolution grid discretization of vertical layers to satisfy the requirement in the hybrid discrete-continuum modeling method. However, conduit diameters sometimes can be extremely large in the field, especially the horizontal segments and the outlets of the conduit network near the surface. For example, the large conduit diameters are about 20–30 ft in average in the Upper Floridan Aquifer (UPA) of the Woodville Karst Plain (WKP), north Florida. Some can be as large as 50 ft or even 100 ft at the outlet of a conduit system, where seawater siphons into the conduit or freshwater discharges into the sea [*Kernagis et al*., 2008; *Kincaid and Werner*, 2008; *Gallegos et al*., 2013]. The UPA with 400 ft in total thickness is vertically discretized as multiple layers, for example, 40 layers with 10 ft thickness in each layer to accurately simulate density-dependent vertical flux. At the same time, the maximum conduit diameter in the variable-density discrete-continuum model can be only 1–2 ft, which is required to be about one order of magnitude smaller than the grid cell thickness. Therefore, the contradiction between large conduit geometries in the field versus the high-resolution grid thickness and even smaller conduit diameter is a big challenge to the VDFST-CFP model. The constant density discrete-continuum numerical model has the capability to simulate flow and solute transport through large conduit diameter without this issue, since its vertical grid discretization does not have to be very small. The entire aquifer is vertically discretized as only one or two layers in many previous discrete-continuum modeling studies [*Gallegos et al*., 2013; *Kuniansky*, 2014; *Xu et al*., 2015a, 2015b]. The two VDSFT-CFP benchmark cases and other testing cases show that the ratio of conduit diameter and grid thickness significantly determine the mass balance discrepancy. Mass balance discrepancy in the VDFST-CFP model increases dramatically and becomes unacceptably large, when the ratio of conduit diameter and grid thickness increases over the criteria.

The applied numerical methods significantly impact the model uncertainty and accuracy as well. Numerical solution of the advection-dispersion equation is relatively expensive in computational cost, since the first derivative term (advection) and the second derivative term (dispersion and diffusion) coexist in the solute transport governing equation [*Zheng and Wang*, 1999]. To keep the numerical method implementation simple and consistent in the code, the finite difference method is used in the VDFST-CFP model to solve the advection-dispersion solute transport equation in both the conduit and the porous medium. Several other numerical methods are optional for solving transport equations in MT3DMS, such as the Eulerian standard finite difference, the mixed Eulerian-Lagrangian, and the third-order TVD (Total Variance Dimishing) method [*Zheng and Wang*, 1999], but are not used in the VDFST-CFP model. The solution of advection transport is first-order accurate by the finite difference method, which could lead to significant numerical dispersion error when solute transport becomes advection-dominated [*Zheng and Wang*, 1999]. *Zheng and Bennett* [2002] pointed out that the finite difference method in solute transport simulation requires that the Peclet number (P_e) to be smaller than 4 for an accurate solution without numerical stability and mass balance issues. The Peclet number (P_e) is defined as:

$$P_e = \frac{|v|L}{D} \leq 4 \quad (27)$$

where v is the seepage velocity [LT^{-1}]; L is the characteristic length, commonly taken as the grid cell width [L]; and D is the dispersion coefficient [L^2T^{-1}].

In the salt transport part of the VDFST-CFP model, each conduit tube is discretized into 10 segments for solving the advection-dispersion equation by finite difference method. The sub-discretization of conduit network is necessary to decrease the Peclet number in the solute transport simulation with rapid conduit flow. On the other hand, because of the relatively large exchange permeability on the conduit wall and matrix hydraulic conductivity, the groundwater seepage velocity in the surrounding porous medium is accelerated by the dynamic exchange from the conduit system. Therefore, the solute transport process easily becomes advection-dominated in the porous medium near the conduit network, and the Peclet number may exceed the numerical stability criteria required by the finite difference method. In other words, simulation result can be inaccurate with large truncation error when solute transport becomes advection-dominated in parts of the porous medium near the conduit system. The high-resolution grid discretization and small layer thickness are desired for a smaller Peclet number. Generally speaking for the VDFST-CFP model, the physical dispersivity should be large enough or the grid spacing should be sufficiently small, which would significantly increase the computational cost.

In the horizontal and vertical benchmark studies, the continuum SEAWAT and MODFLOW/MT3DMS models are compared with the discrete-continuum CFPv2/UMT3D model and the newly developed VDFST-CFP model. The equivalent values of conduit diameter and friction factor in the discrete-continuum models are calculated from the hydraulic conductivity of conduit network in the continuum model using the methods introduced in section 3.1. The Darcy equation (equation 25) is used in the continuum model with an assumption of the linear relationship between specific discharge and hydraulic gradient. The Hagen-Poiseuille equation (equation 24) is applied in a cylindrical conduit with the estimations of the friction factor and the Reynolds number under laminar flow condition. The combination of the Hagen-Poiseuille and Darcy equations generate the equivalent relationship of hydraulic conductivity respect to the conduit diameter under laminar flow condition, but its uncertainty for conduit flow under turbulent flow condition is unknown. The Darcy equation does not provide an appropriate solution for nonlaminar groundwater flow, and significantly overestimates the conduit flow under turbulent flow condition. The friction factor is also underestimated with a larger Reynolds number under turbulent flow condition. The relationship between the friction factor and the Reynolds number under turbulent flow condition can be approximated using the Blasius estimation or the Colebrook-White equation. However, neither the Blasius estimation nor the Colebrook-White equation can be combined with the Darcy-Weisbash equation to derive a simple relationship between equivalent turbulent hydraulic conductivity and conduit diameter without the flow velocity or the Reynolds number. Although the friction factor is not solely a function of conduit wall roughness, equivalent hydraulic conductivity is a constant physical parameter of the conduit system. Therefore, in the benchmarks of the VDFST-CFP model in this study, equivalent hydraulic conductivity under turbulent flow condition is assumed as same as that under the laminar flow condition. The assumption is believe to be reasonable, since the overestimation of flow rate by the Darcy equation would be offset with the overestimation of friction factor under turbulent flow condition, although the quantitative uncertainty of this approximation is hard to estimate.

Two categories of convergence criteria are important in the VDFST-CFP model for the mass balance discrepancy and simulation accuracy. The convergence criterion for the Newton-Raphson method determines the numbers of iteration loops for solving conduit flow solution in the density-dependent Darcy-Weisbach equation, and also controls the accuracy of head and flow rate calculations in the conduit system. The convergence criteria of implicit coupling approach are important for simulation accuracy as well. The discrepancies in head solution are relatively small, but can be large in solute transport sometimes. The convergence criteria of head and density in the conduits are smaller and more sensitive than those used in the porous medium, for example, the maximum differences of head (0.0001 ft) and density (0.00002 lb/ft^3) from the previous loop in the conduit, respectively. In addition, the time step size and the spatial discretization of grid cell size also significantly affect the numerical stability, simulation accuracy and mass balance.

5 Conclusion

In this study, the discrete-continuum numerical model (VDFST-CFP) is developed to simulate density-dependent nonlaminar and laminar groundwater flow and salt transport in a conduit and the surrounding porous medium. The newly developed VDFST-CFP model provides a quantitative simulation of seawater/freshwater mixing process in a coastal karst aquifer, especially seawater intrusion into the subsurface conduit network. The concept of equivalent freshwater head is used in the variable-density groundwater flow governing equations with additional density terms. Laminar groundwater flow in the porous medium is simulated by the Darcy equation. The density-dependent Darcy-Weisbash equation is applied to simulate nonlaminar groundwater flow in the conduit, because conduit flow rate is nonlinear to hydraulic gradient. Conduit-matrix water exchange rate is assumed linear to the head difference between the two domains. Salt transport is governed by the advection-dispersion equation with flow simulation results in both domains. Groundwater flow in the continuum porous medium and solute transport equations are numerically solved by the finite difference method. The density-dependent Darcy-Weisbash equation is derived in this study and solved iteratively for the conduit flow rate by the Newton-Raphson method. Groundwater flow and solute transport solutions in the conduit and porous medium are coupled by an implicit iterative procedure within each time step.

Two VDFST-CFP benchmarks are setup and compared with other commonly used numerical models, including variable-density SEAWAT, constant density continuum MODFLOW/MT3DMS, and discrete-continuum CFPv2/UMT3D models. The horizontal benchmark investigates the discrete-continuum hybrid modeling method, and the vertical benchmark evaluates the density-dependent flow and transport simulation. Horizontal flux is not density-dependent, and the results of variable-density models are similar to the constant density models in the horizontal benchmark. The Darcy equation overestimates the conduit flow rates under turbulent condition, and the simulated salt plumes in the continuum models extend significantly further landward. In the vertical benchmark, the simulation results of both two models are similar to each other, because the Darcy equation in the SEAWAT model does not overestimate the flow rate of relatively slow conduit flow rate. Parameter sensitivity analysis results indicate conduit diameter and friction factor are important to seawater intrusion in both the conduit and porous medium domains. Conduit wall permeability does not significantly impact the mixing zone position, at least in the two benchmark studies with small head difference between the domains. The large hydraulic conductivity in the porous medium and the exchange permeability accelerate the conduit flow, but dilute the salinity plume and decrease the peak of salinity in the porous medium due to strong dispersion. The effective medium porosity is also an important parameter to the salt transport and mixing zone position in the porous medium, but rarely affects simulation results in the conduit.

The VDFST-CFP model has critical limitations to its uncertainty, instability, and accuracy issues. First, the combination of variable-density flow model and discrete-continuum modeling method requires sufficient high-resolution vertical discretization of porous medium and small conduit diameter within the grid cell. This restriction is contradicted to the giant conduit dimension in many karst aquifers, therefore limited the applications of the VDFST-CFP model to many field cases. The numerical stability and simulation accuracy can be significantly improved with smaller ratio of conduit diameter and grid cell. Second, the advection-dispersion transport equation is solved by the finite difference method in the VDFST-CFP model, which possibly generates large truncation error for advection-dominated transport in the porous medium near the conduit system, especially under turbulent flow condition. Third, in the model comparison among different models, the equivalent relationship between conduit diameter and hydraulic conductivity of the conduit system is made under laminar flow condition. The equivalent hydraulic conductivity is set constant in the continuum models, but its uncertainty in a non-laminar flow condition is unknown. In addition, the Newton-Raphson method and the implicit iterations convergence criteria significantly affect the model accuracy and mass balance discrepancies.

Overall, this study develops the novel VDFST-CFP model to simulate density-dependent seawater intrusion in the conduit and the porous medium domains, using the hybrid discrete-continuum modeling method. However, further developments are still necessary to relax the limitations of VDFST-CFP, then which can be applied to real fields. Parallel computing and reduced order model techniques will be useful to save computational cost and speed up the simulation. The numerical dispersion and truncation errors probably can be diminished by using some other numerical methods for solving the differential equations, such as finite element, finite volume, and the TVD methods. Additional works are required to solve the numerical stability issues and improve the simulation accuracy in the current VDFST-CFP model.

Acknowledgments

The authors would like to thank Barclay Shoemaker at USGS Florida Water Science Center, Thomas Reimann at TU Dresden and Weixing Guo at Schlumberger Water Services for providing helpful insights and comments during the numerical model development. Marilyn Saarni at Lawrence Berkeley National Laboratory helped to polish the manuscript and provided many revision suggestions in English editing. Eve Kuniansky, two anonymous reviewers and WRR editors provide important reviews for this paper. This project is partially funded by National Natural Science Foundation of China (NSFC) (grant 41530316, 91125024), the National Key Research and Development Program of China (grant 2016YFC0402805), and Lawrence Berkeley National Laboratory LDRD project 103912. The VDFST-CFP source codes and model files can be obtained by contacting the authors: Zexuan Xu (xuzexuan@gmail.com) or Bill Hu (bill.x.hu@gmail.com).