2017

Numerical Simulation of Seawater Intrusion in a Well-Developed Coastal Karst Aquifer by Using VDFST-CFP Model

Zhongyuan Xu
NUMERICAL SIMULATION OF SEAWATER INTRUSION IN A WELL-DEVELOPED COSTAL KARST AQUIFER BY USING VDFST-CFP MODEL

By

ZHONGYUAN XU

A Thesis submitted to the
Department of Earth, Ocean and Atmosphere Science
in partial fulfillment of the
requirements for the degree of
Master of Science

2017
Zhongyuan Xu defended this thesis on June 1, 2017.

The members of the supervisory committee were:

Xiaolong Hu
Professor Directing Thesis

Yang Wang
Committee Member

Stephen Kish
Committee Member

Ming Ye
Committee Member

The Graduate School has verified and approved the above-named committee members, and certifies that the thesis has been approved in accordance with university requirements.
This Thesis is dedicated to my family.
ACKNOWLEDGMENTS

It could be a stage achievement for me to get a master degree at Florida State University, but I would not end up my college study and academic career. I am thankful for the path I have taken and more importantly for the people that have lined this way. I would like to acknowledge the people listed below for helping me achieve my goals.

Let me begin by expressing sincere gratitude to my major professor Dr. Bill Hu for giving me this opportunity to do my graduate study at FSU. Dr. Hu changed my entire life goal to pursue hydrogeology and groundwater modeling. In the whole study, Dr. Hu steered me in the right direction and talked me off the ledge often. I also want to appreciate my committee members: Dr. Ming Ye, Dr. Stephen Kish and Dr. Yang Wang. Dr. Ye taught me a lot about numerical modeling and scientific thinking; Dr. Kish instructed me with the local karst environment and involved me into the laboratory experiments; Dr. Wang aroused my interest in the application of geochemistry on the hydrogeology. As well as, I would like to thank Dr. Zexuan Xu, who provided me numerous assistance and patient guidance on my thesis research and coding problems.

In addition, I hope to express my gratitude to Osmond Tanner Endowment and the selection committee, I was excited to be a selected recipient of this honor, and I am truly appreciate your financial support. I also want to thank many professors who provide significant helps in my study and research, including Dr. James Tull, Dr. Williams Park, Dr. Leroy Odom and Dr. David Farris.

Furthermore, I received a lot of help from my friends and roommates, they are Ruiguang Pan, Jin Liu, Xingqiang Chen, Xin Shan, Canlin Zhang, Shuying Yang, Yanxia Li, Haibin Hang, Zhongjun Hu, Tian Nan, Kassandra Derf, Andrew Stevens and Rupsa Roy, thank you very much in this two years.

Last, I would like to express my great gratitude to my family members, my mother Ruolan Xu, my father Yaping Zhang, my brother Yaoyuan Zhang and my girlfriend Xiujie Wu. Thank you for providing me enough support and giving me huge love, I love you all.
# TABLE OF CONTENTS

LIST OF TABLES .......................................................................................................................... vi

LIST OF FIGURES ....................................................................................................................... vii

ABSTRACT ................................................................................................................................... ix

1. INTRODUCTION AND BACKGROUND ............................................................................... 1
   1.1 Seawater intrusion in karst aquifer ....................................................................................... 1
   1.2 Woodville Karst Plain (WKP) hydrologic study ................................................................. 3
   1.3 VDFST-CFP ......................................................................................................................... 6

2. VDFST-CFP GOVERNING EQUATION AND METHODS ................................................. 10
   2.1 Variable density flow in porous media ............................................................................... 11
   2.2 Solute transport in porous media ........................................................................................ 13
   2.3 Variable-density groundwater flow in karst conduits ......................................................... 13
   2.4 Solute transport in karst conduits ........................................................................................ 16
   2.5 Roughness of conduits ........................................................................................................ 17

3. NUMERICAL MODEL SETUP .............................................................................................. 23
   3.1 Conceptual model ............................................................................................................... 23
   3.2 Model domain ..................................................................................................................... 23
   3.3 Boundary conditions and initial conditions ....................................................................... 25
   3.4 Hydraulic properties ........................................................................................................... 25
   3.5 Simulation results ................................................................................................................ 26
   3.6 Parameter sensitivity study ................................................................................................. 27

4. SENSITIVITY ANALYSIS ..................................................................................................... 31
   4.1 Methodology ....................................................................................................................... 31
       4.1.1 Local sensitivity analysis .............................................................................................. 31
       4.1.2 Global sensitivity analysis with Morris Method ........................................................... 32
   4.2 Local sensitivity analysis .................................................................................................... 33
   4.3 Global sensitivity analysis .................................................................................................. 35
   4.4 Discussion of sensitivity analysis ....................................................................................... 37

5. SCENARIOS STUDY .............................................................................................................. 42
   5.1 Salinity variation at the submarine spring .......................................................................... 42
   5.2 Sea level variation ............................................................................................................... 44

6. CONCLUSION ......................................................................................................................... 47

REFERENCES ............................................................................................................................. 49

BIOGRAPHICAL SKETCH ........................................................................................................... 54
LIST OF TABLES

Table 4.1 Parameter values of the conduit and porous media in the VDFST-CFP model .......... 26

Table 4.2 The specified values of local analysis and value ranges of global analysis of seven parameters, the parameters are cited from Xu et al. (2017a) and Davis et al. (2010) ................. 33

Table 4.3 The specified values of local analysis and value ranges of global analysis of adjusted parameters ............................................................................................................................ 38
LIST OF FIGURES

Fig 1.1 (a) Locations of the Woodville Karst Plain and the study site; (b) Map of the Woodville Karst Plain, showing the locations of features of note within the study area; (c) Locations of Falmouth 2D-ACM meters and Wakulla Spring cave system; (d) Locations of Spring Creek Spring vents, from Lane 21; (e) Groundwater elevation profile in major karst windows grouped by Spring Creek salinity, from 22. Figure 1.1 a–c were created using ArcMap version 10.3.1, copyright and licensed by ESRI, http://desktop.arcgis.com/en/; (d) is a reprint from Lane 21; (e) was created using R version 3.2.3, licensed under GNU Public License 2&3 (GPL-2&3), https://www.R-project.org/. All maps and data in figures were created using data acquired by the State of Florida those are also in the public domain and not subject to copyright. (Xu et al., 2016) ................................................................. 5

Fig 1.2 Schematic figure of finite difference grid discretization and boundary conditions applied in the horizontal and vertical benchmark cases (Xu and Hu, 2016b; 2016c). (a) is horizontal benchmark case; (b) is vertical benchmark case................................................................. 7

Fig 1.3 Salinity simulation results by the two continuum numerical model and the other two discrete-continuum numerical model in the horizontal case: (a) SEAWAT (upper left); (b) MODFLOW/MT3DMS (upper right); (c) CFPv2/UMT3D (lower left); (d) VDFST-CFP (lower right). The unit of concentration is PSU (Practical salinity units). ................................. 8

Fig 1.4 Salinity simulation results by two density-dependent numerical models in the vertical case: (a) SEAWAT (upper); (b) VDFST-CFP (lower) (Xu and Hu, 2016c). The unit of concentration is PSU (Practical salinity units)................................................................. 9

Fig 2.1 Geometry and flow direction of convergence point. ........................................................ 16

Fig 2.2 The cave and rock stacking in the extensive karst conduit can be replaced by expansion and contraction in the model: (a) is karst conduit with cave and falling rocks; (b) is conduit wall with an expansion; (c) is conduit wall with a contraction. L1 is the length before the component [L], L2 is the length of the component [L], L3 is the length after the component [L]; D is the diameter of conduit [L]; De is the diameter of expansion part [L]; Dc is the diameter of contraction part [L]; V1 is the flow velocity before the component [LT-1], V2 is the flow velocity at the component [LT-1], V3 is the flow velocity after the component [LT-1]................................................................................................................. 20

Fig 3.1 Schematic cross-section of a coastal karst aquifer with conduit networks and submarine spring. Flow direction would be seaward when precipitation recharge is large; however, reversal occurs when sea level rises, pumping rate is higher or precipitation recharge is smaller.......................................................................................................................... 23

Fig 3.2 Schematic finite difference grid discretization and boundary conditions applied in the vertical benchmark case. represents porous media; represents conduit system; represents sea water boundary, the constant head is 0.0 ft and constant concentration is 35.0
PSU at sea water boundary; ■ represents fresh water boundary, where constant head is 5.0 ft and constant concentration is 0.0 PSU.

Fig 3.3 Salinity simulation in VDFST-CFP model. (a) is seawater intrusion in single-pipe model; (b) is seawater intrusion in multi-pipe model; (c) is seawater intrusion in double-pipe model. Yellow represents high concentration, blue represents low concentration.

Fig 3.4 The effect of parameters variation on seawater intrusion, the plots on the left column are the simulations in the conduit, the plots on the right column are the simulations in the matrix (layer #20).

Fig 4.1 CSS values in conduit. Upper plot is the total, salinity and head CSS values of seven parameters to conduit simulation; lower plot is the total CSS values at different locations along conduit.

Fig 4.2 CSS values in matrix (layer #20). Upper plot is the total, salinity and head CSS values of seven parameters to simulations; lower plot is the total CSS values at different locations along conduit.

Fig 4.3 Mean and standard deviation of element effect of each parameter: (a) salinity in the conduit; (b) head in the conduit; (c) salinity in the matrix; (d) head in the matrix.

Fig 4.4 Results of new local sensitivity analysis: (a) total, salinity and head CSS values of seven parameters to conduit simulation; (b) total CSS values at different locations along conduit; (c) total, salinity and head CSS values of seven parameters to matrix simulation (Layer 20); (d) total CSS values at different locations along Layer 20.

Fig 4.5 Mean and standard deviation of element effect of each parameter in new global sensitivity analysis: (a) salinity in the conduit; (b) head in the conduit; (c) salinity in the matrix; (d) head in the matrix.

Fig 5.1 Salinity distribution under different salinity conditions at submarine spring which indicates various precipitation and freshwater discharge: from top to bottom, they are 0.0 PSU, 10.0 PSU, 20.0 PSU, 30.0 PSU at the submarine spring.

Fig 5.2 Position of mixing zone in the matrix and conduit, average salinity in conduit system under various salinity at submarine spring, position of mixing zone is the rightmost cell which salinity is larger than 10 PSU in the Fig 5.1.

Fig 5.3 Salinity distribution under different sea levels: from top to bottom, they are -1.0 ft, -0.5 ft, 0.5 ft, 1.0 ft, the result of 0.0 ft is displayed in Fig 3.3(a).

Fig 5.4 Position of mixing zone in the matrix and conduit under various sea level, position of mixing zone is the rightmost cell which salinity is larger than 10 PSU in the Fig 5.3.
ABSTRACT

Well-developed karst aquifers contain high permeability limestone matrix and much higher conductive conduits, this dual porosity system behaves totally different from other kinds of aquifers and becomes a challenging task for modern hydrogeological study. High permeable conduit system provides idea pipes for contaminant transporting in rapid flowing groundwater, this effect may cause wide range pollution in a short time. One of these serious problems is seawater intrusion. Seawater intrusion has been found in many coastal aquifers, produced contaminated fresh groundwater resources and induced ecosystem problems. Seawater intrusion in a well-developed karst aquifer such as Woodville Karst Plain (WKP) is simulated by Dr. Zexuan Xu (Xu and Hu, 2017a), he developed a new model VDFST-CFP (Variable-Density Flow and Solute Transport - Conduit Flow Process) which considers the variable density flow in dual porosity system.

VDFST-CFP provides an accurate simulation of seawater intrusion in a coastal karst aquifer with conduit networks. It couples the variable density flow field and the density function of salinity in the porous medium and non-laminar groundwater flow within karst conduits. Currently, the VDFST-CFP model is used to simulate seawater intrusion condition at a synthetic level, the present numerical simulation only considered the idea circumstance that is one conduit in a 2D model, and data analyses mainly focused on the horizontal source.

In this study, an improvement of VDFST-CFP will concentrate on the vertical source model in the WKP, the roughness of conduit wall and multiple pipes will be considered. Two improvement are implemented in the new model: (1) multi-conduit networks in the domain; (2) micro- and macro-structures on the conduit wall (conduit wall roughness). The simulation results show that dual-pipe system produced a larger contaminant plumes than single-pipe system. Meanwhile, rougher micro-structures and more macro-structures on conduit wall slow down the velocity of seawater intrusion in conduit system, however, have a limited affect salinity distribution in the matrix. In addition, local sensitivity analysis and global sensitivity analysis of seven parameters (conductivity, diameter, dispersivity, exchange permeability between conduit and matrix, effective porosity, mean roughness height and specific storage) are conducted in this study. Sensitivity results indicate that conductivity, diameter and porosity are more important to head and salinity distribution simulations than other four parameters. Diameter is the most
important parameter to the conduit simulation, while matrix simulations is more sensitive to effective porosity. Furthermore, scenarios study about variation of boundary conditions is conducted, the result shows that a decreasing of salinity at submarine spring or a decreasing on sea level moves seawater intrusion backward both in conduit and matrix, while the intrusion in conduit and matrix have different sensitivities to the change of boundary conditions.
CHAPTER ONE
INTRODUCTION AND BACKGROUND

Karst aquifer systems underlie approximately 10-20% of Earth’s landmass and supply portable water to nearly 25% of the world’s population (Ford and Williams, 1989). About 15% of the conterminous United States has carbonates, gypsum or other soluble rocks at the land surface and nearly 25 million cubic meters of water per day is withdrawn from carbonate aquifers in America (Peck et al., 1988). However, carbonate aquifers are commonly vulnerable to contamination from surrounding environment. Seawater intrusion is one of the severe environmental problems in the coastal karst aquifer, such as Woodville Karst Plain. In this paper, Woodville Karst Plain was selected as the study site to investigate the numerical simulation of seawater intrusion.

1.1 Seawater intrusion in karst aquifer

Sea level rise has been widely recognized as a global environmental threat associated with climate change and global warming (Bear et al., 1999; IPCC, 2007; FitzGerald et al., 2008). Fresh groundwater in coastal regions can be significant influenced by salt water associated with the process of sea level rise, this process is usually described as seawater intrusion. Seawater intrusion causes several serious challenges such as soil salinization, marine and estuarine ecological change, and groundwater contamination (Bear, 1999). Inland water resources and ecological systems are extremely vulnerable to the seawater intrusion, especially coastal karst aquifers. Salt water transport in conduits are much faster than in porous media, this process is significant complex since an underground conduit system is difficult to accurately explore and measure, and may give rise to long-distance seawater intrusion that can affect further upstream aquifer. Some studies (Arfib et al., 2006; Fleury et al., 2007; Davis and Verdi, 2014) has indicated that the seawater intrusion occurs at the submarine karstic springs where salt water backflows into, most of these submarine-spring-intrusions are seasonal functioning such as Spring Creek Springs in Woodville Karst Plain. Davis and Verdi (2014) summarized the fresh water and seawater cycling in the WKP, concluded the seawater intrusion is sensitive to the climate change and precipitation. Xu et al. (2016a) illustrated the longest documented seawater intrusion which migrates 14 miles inland to Wakulla Spring (one of Florida’s major first magnitude springs). The composite analysis of
precipitation, electrical conductivity data from 2D-ACM flowmeters and geochemical data in this paper provided strong evidence to support Davis’ conclusion.

Groundwater flow in karst conduits is different from that in surrounding matrix, Darcy’s law is no longer suitable for these dual-permeability situations. Some researchers (Bakaloxicz, 2005; Gallegos et al., 2013) have conducted numerical dual-permeability models to study groundwater flow and solute transport in a well-developed karst aquifer. Shoemaker et al. (2008) developed the MODFLOW-CFP by coupling groundwater modeling code MODFLOW (Harbaugh et al., 2000; 2005) which is based on Darcy’s law to simulate laminar flow in porous media. CFP (Conduit Flow Process) considers the transition of laminar flow and turbulent flow by Reynolds number and solves the turbulent flow rate in conduits by using Darcy-Weisbach equation. Reimann et al. (2011; 2013; 2014) enhanced CFP by adding conduit associated drainable storage (CADS) and time-variable boundary condition, and developed CFPv2 which enabled solute and heat transport modeling in karst aquifer. Xu et al. (2015a; 2015b) used CFPv2 developed the Nitrate-N distribution and seawater intrusion in WKP which considered the solute transport in karst conduits.

In addition, groundwater flow containing dissolved constituents may affect fluid density. When solute concentration is minimal, the effect of density is negligible and Darcy’s law is suitable for the groundwater modeling in matrix field; however, as solute concentration increases such as in a coastal aquifer, the governing equation has to be changed, a variable-density groundwater model is needed. The variable-density groundwater theory has been studied for a long time during last two centuries (Ghyben, 1888; Herzberg, 1901; Hubbert, 1940; Pinder and Cooper, 1970; Voss and Souza, 1987; Croucher and O’Sullivan, 1995), some numerical coupling models also have been used in variable-density groundwater modeling, such as SUTRA (Voss, 1984), MOCDENSE (Sanford and Konikow, 1985) and HST3D (Kipp, 1997). SEAWAT (Guo and Langevin, 2002; Langevin et al, 2003; 2008) is the most popular numerical code for variable-density groundwater flow and solute transport, MODFLOW (Harbaugh et al., 2000) is applied to govern the groundwater flow by finite difference method and MT3D (Zheng and Wang, 1999) is used to solve the solute transport within SEAWAT. However, SEAWAT is only applicable for groundwater flow in porous media. For simulating salt water flow in karst aquifer with conduits, a new numerical code which couples dual-permeability flow modeling and variable-density flow modeling need to be established, Xu and Hu (2016b; 2016c) developed VDFST-CFP to make an attempt in this domain of science.
1.2 Woodville Karst Plain (WKP) hydrologic study

The Woodville Karst Plain is located in north Florida, covers about 500 square miles and extends from the Cody Scarp and Tallahassee south to the Gulf of Mexico (Fig 1.1). The geology of the WKP consists of a thin veneer of unconsolidated and undifferentiated Pleistocene quartz sand and shell beds overlaying a thick sequence of relatively horizontal carbonate rocks that comprise the Upper Floridan Aquifer (UFA) (Kincaid et al., 2005). According to Bush and Johnson (1988), the elevation in the WKP generally range from 0 to 35 ft above mean sea level, with a trending slope of less than 4 ft per mile southward to Gulf. The precipitation is relatively high with humid climate, the average annual temperature and precipitation are about 67 ºF and 66 inches per year separately. The average yearly potential evapotranspiration for Tallahassee area is estimated to be about 46 inches per year (Smajstrla et al., 1984).

Karst features can be illustrated from a geologic point of view. In the UFA, the St. Marks Formation in Miocene sediments is primarily a fine to medium grained, silty to sandy limestone that has undergone varying degrees of secondary dolomitization (Hendry and Sproul, 1966), permeability can range from highly permeable to relatively impermeable. The Oligocene Suwannee Limestones is beneath the St. Marks Formation and generally permeable to very permeable. Under Oligocene sediments, the Eocene sediments also consist of permeable limestone (Miller, 1986). The permeability of the UFA is directly related to the thickness and lithology of the overlying low-permeability sediments (Davis et al., 2010). During Pleistocene, these low-permeability sediments removed leads to current karst distribution and present transmissivity which ranges from $1.3 \times 10^3$ to $1.3 \times 10^6$ feet squared per day (Davis, 1996).

The largest discharge surficial spring is Wakulla Spring with an average discharge of 380 cubic feet per second, seasonal discharge from Wakulla Spring ranges from 25.2 to 1910 cubic feet per second (Scott et al., 2002). Wakulla Spring is located 11 miles upstream from the coastal shoreline of Gulf of Mexico, it is the headwaters of the Wakulla river which is 14.3 miles discharging into the sea. The elevation at Wakulla Spring is normally around 5.0 ft above sea level, which is significant to the determination of conduit water flow direction and hydraulic connection between other discharging springs. Groundwater flow through Wakulla Spring by an extensive submerged cave systems (Loper et al., 2005). Cave divers have explored these cave system from Wakulla Spring and other sinkholes since 1987, various interconnected tunnels have been
identified by the cave explorers. The depth of Wakulla conduit system is estimated to be 200ft near the vent, extended to 300 ft and could be 360 ft along portions of the system (Florida Springs Task Force, 2000). However, the groundwater flow and conduit connection in Wakulla Spring springshed has not been fully described.

The major submarine spring in the coastal portion of the study area is Spring Creek Springs system, it consists of 14 submarine spring vents opening into the Gulf of Mexico. However, the exact locations of vents are difficult to explore and survey since they exist in the depths of the bay. Spring Creek Springs is a type 2 submarine spring as illustrated by Fleury et al. (2007), type 2 springs have well-developed karst networks and possess valuable storage capacities. The flow rate of these springs is typically high and strongly depends on seasonal variability, this characteristic causes salinity of water to be low during high flow rate and increases when flow rate decreases. During times of drought when rainfall and surface recharges are low, the pressure of freshwater is too weak to prevent seawater flow into conduits. Davis and Verdi (2014) developed a conceptual model to explain the cycling of freshwater and seawater flows in Spring Creek Springs, they divided groundwater flow into 3 phases. Phase 1: during an extended period of low rainfall, the surface water recharges decreasing allows seawater to move landward and backflow into the aquifer through the Spring Creek Springs. The submarine caves are filled with salt water and block the freshwater discharge. Due to the density difference between the salt water and fresh water, the equivalent fresh water head in Spring Creek Springs can reach 7.5 ft, while the river stage and hydraulic head of Wakulla Spring is about 5 ft. The groundwater prefers to discharge at the inland springs rather than coastal vents. Phase 1 is the typical seawater intrusion, the literature review of seawater intrusion is introduced in Section 2.2; Phase 2: A high rainfall event generates a large amount of surface water recharge into aquifer. The blockage of fresh water flow by salt water at the Spring Creek Springs during Phase 1 causes an increase in gauge height at Wakulla Spring. Finally, the seawater is pushed out and replaced with freshwater, the equivalent fresh water head is no longer 7.5 ft, which should be the altitude of sea level or tidal level; Phase 3: Rainfall returns to normal condition, the Spring Creek Springs continue to discharge fresh water but the groundwater level in the UFA gradually drops with the storage reduction, the low water level in aquifer becomes more and more vulnerable to seawater intrusion. Phase 3 may last a long time until the seawater moves upstream into conduits again during subsequent droughts.
Fig 1.1 (a) Locations of the Woodville Karst Plain and the study site; (b) Map of the Woodville Karst Plain, showing the locations of features of note within the study area; (c) Locations of Falmouth 2D-ACM meters and Wakulla Spring cave system; (d) Locations of Spring Creek Spring vents, from Lane 21; (e) Groundwater elevation profile in major karst windows grouped by Spring Creek salinity, from 22. Figure 1.1 a–c were created using ArcMap version 10.3.1, copyright and licensed by ESRI, http://desktop.arcgis.com/en/; (d) is a reprint from Lane 21; (e) was created using R version 3.2.3, licensed under GNU Public License 2&3 (GPL-2&3), https://www.R-project.org/. All maps and data in figures were created using data acquired by the State of Florida those are also in the public domain and not subject to copyright. (Xu et al., 2016)
Numerical simulations are another prevalent method to study Woodville Karst Plain. Davis et al. (2010) conducted a groundwater flow and contaminant transport modeling to simulate the effect of nitrate-N sources on Wakulla Spring springshed by the coupling of MODFLOW and MT3DMS. Their simulation derived the nitrate distribution from 1966 and predicted to 2018. The results show the nitrate-N load decreases at the contaminant source due to the planned reduction in the concentration of nitrate used in irrigation; while the nitrate-N load rises at Wakulla Spring system respective to the increases in population and residential and commercial sites. This simulation regards karst conduits as high permeable and conductivity zones, however, the groundwater moves in conduits is much more complex than this assumption. Based on the Davis’s model, Gallegos et al. (2013) used MODFLOW-CFP to simulate the groundwater flow in WKP which fully consider the non-laminar condition of water flowing in conduits, the results show MODFLOW-CFP model is closer to the observed data at Wakulla Spring and Spring Creek Springs than MODFLOW model, while the solute transport is not included in Gallegos’ study. Additionally, Xu et al. (2015a) updated the nitrate-N simulation study in WKP by using CPFv2, which both considers the non-laminar flow and solute transport in conduits, a more accurate and accepted result is concluded in Xu’s paper.

1.3 VDFST-CFP

VDFST-CFP is a hybrid discrete-continuum numerical model for simulating variable-density groundwater flow and solute transport in conduit/matrix dual permeability region, mainly be used in seawater intrusion in a coastal karst aquifer with a conduit network. Density-dependent Darcy-Weisbach equation is developed to describe the groundwater flow in the conduit which is solved in Newton-Raphson method iteratively. The groundwater flow and solute transport equations in matrix are the same as those in SEAWAT; the solute transport in conduits and exchange equations of water and solute between conduits and porous media are similar to the CPFv2. The details of governing equations are included in next section. Two 2D synthetic cases, horizontal benchmark and vertical benchmark (Fig 1.2) of VDFST-CFP are established by Xu and Hu (2016b; 2016c).
The results of models were compared with compatible SEAWAT and other numerical code model results to verify the reasonable of VDFST-CFP (Fig 1.3; Fig 1.4). The results of parameter sensitivity analysis focus on horizontal model indicates the conduit diameter, friction factor and hydraulic conductivity are important for this model. However, the VDFST-CFP model is still in the primary stage, the prerequisite assumption of this model is too rigor to use it in the real case. This thesis will continue improving this model based on Dr. Xu’s previous study, the major governing equations of VDFST-CFP will not be changed.
Fig 1.3 Salinity simulation results by the two continuum numerical model and the other two discrete-continuum numerical model in the horizontal case: (a) SEAWAT (upper left); (b) MODFLOW/MT3DMS (upper right); (c) CFPv2/UMT3D (lower left); (d) VDFST-CFP (lower right). The unit of concentration is PSU (Practical salinity units).
Fig 1.4 Salinity simulation results by two density-dependent numerical models in the vertical case: (a) SEAWAT (upper); (b) VDFST-CFP (lower) (Xu and Hu, 2016c). The unit of concentration is PSU (Practical salinity units).
CHAPTER TWO

VDFST-CFP GOVERNING EQUATION AND METHODS

Numerical computation of seawater intrusion is variable-density flow and solute transport issue, the flow field and transport equations have to be solved under implicit iterative procedure both in porous media and karst conduits. In the VDFST-CFP modeling, the groundwater flow field equation is solved by using the water density that is determined by the salinity of the last step, then the concentration of salt is calculated by the flow field and then used in the next step. This iterative process is repeated within each time step until the consecutive change in fluid density is less than a convergence value. The computational cost in the implicit iteration is very large in this model, in order to reduce the coding effort and computational burden, as well as make the model representativeness and keep the model reasonable and guarantee the model accuracy, some assumptions are necessary and listed below:

1) The model is two-dimensional with one or more conduits in the network. The computational cost for three-dimensional model will be unaffordable. The code could be extended into three-dimensional and multiple conduits in future studies with parallel computing technique.

2) The aquifer is confined and the conduit is fully saturated. The governing equations and numerical implementation of groundwater flow in a confined aquifer are much simpler than that in an unconfined aquifer with variable thickness and transmissivity. The subsurface conduit network is usually existed in the deep coastal karst aquifer to avoid the complex calculation of variable saturation condition, for example, the karst conduit networks in the Woodville Karst Plain (WKP), north Florida, where submarine caves are as deep as 285 ft deep under surface.

3) Groundwater viscosity is assumed to be constant. Viscosity is basically dependent on temperature, which is assumed constant in this study as well. Density is a sole function of salinity in this study.

4) Matrix porosity is assumed to be constant. The physical and chemical processes that may change matrix porosity, including carbonate dissolution and precipitation, weathering and erosion, are not considered in this study.
5) The difference between the compressibility coefficients of saline water and freshwater is negligible.

6) The variation of density is linear to salinity. The advection-dispersion of solute transport equation is applied without additional density terms, while the effect of variable density only affects groundwater flow.

7) Darcy-Weisbach equation is directly applied in the groundwater flow simulation in the conduit, whether there are laminar or turbulent conditions. Same as the MODFLOW-CFP simulation, Reynolds number of groundwater flow in the conduit is calculated to determine the flow is either turbulent or laminar in this paper.

8) Micro- and macro-structures are considered in this study, the height of micro-structures is assumed to be less than 5 percent of conduit diameter; the height of macro-structures is assumed to be less than 30 percent of conduit diameter.

\[ 2.1 \text{ Variable density flow in porous media} \]

Harbaugh (2005) illustrated the three-dimensional movement of groundwater of constant density through porous earth media, which is described by the partial difference equation, while in this study, we only consider the two-dimensional modeling:

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

where \( K_{xx}, K_{zz} \) are values of hydraulic conductivity along x and z coordinate axes, which are assumed to be parallel to the major axes of hydraulic conductivity [L/T]; \( h \) is the potentiometric head [L]; \( W \) is a 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].

Guo and Langevin (2002) used equivalent freshwater head to describe variable-density groundwater flow and saline water movement. The conversion between measured head and equivalent freshwater head can be made using the following relations,

\[
h_f = \frac{\rho_s}{\rho_f} h - \frac{\rho_s - \rho_f}{\rho_f} Z \tag{2}
\]

and
where \( h_f \) is the equivalent freshwater head [L]; \( h \) is the measured head [L]; \( \rho_f \) is the density of freshwater [ML\(^{-3}\)]; \( \rho \) is the density of saline groundwater [ML\(^{-3}\)]; \( Z \) is the elevation [L].

Specific discharge or volumetric fluxes of Darcy’s law for a fluid of variable density can be expressed by the equations of,

\[
q_x = -\frac{k_x}{\mu} \frac{\partial P}{\partial x}
\]  \hspace{1cm} (4) \\
and \\
\[
q_z = -\frac{k_z}{\mu} \left( \frac{\partial P}{\partial z} + \rho g \right)
\]  \hspace{1cm} (5)

where \( q_x, q_z \) are the individual components of specific discharge [LT\(^{-1}\)]; \( \mu \) is the dynamic viscosity [ML\(^{-1}\)T\(^{-1}\)]; \( k_x, k_z \) are intrinsic permeability [L\(^2\)] in the two coordinate directions.

The governing equation of Darcy’s Law for variable density flow in terms of equivalent freshwater head would be,

\[
\frac{\partial}{\partial \alpha} \left( \rho K_{f,\alpha} \left[ \frac{\partial h_f}{\partial \alpha} + \frac{\rho - \rho_f}{\rho_f} \frac{\partial Z}{\partial \alpha} \right] \right) + \frac{\partial}{\partial \gamma} \left( \rho K_{f,\gamma} \left[ \frac{\partial h_f}{\partial \gamma} + \frac{\rho - \rho_f}{\rho_f} \frac{\partial Z}{\partial \gamma} \right] \right)
= \rho S_f \frac{\partial h_f}{\partial t} + \theta \frac{\partial \rho}{\partial \gamma} \frac{\partial C}{\partial t} - \bar{\rho} q_s
\]  \hspace{1cm} (6)

where \( \gamma \) represents the direction normal to the bedding, \( \alpha \) represents the principal direction of permeability parallel to the bedding; \( K_{f,\alpha} \) and \( K_{f,\gamma} \) are the freshwater hydraulic conductivities in the \( \alpha \) and \( \gamma \) directions, respectively [LT\(^{-1}\)]; \( S_f \) is the specific storage in terms 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 Solute transport in porous media

Groundwater flow advection, molecular diffusion, and mechanical dispersion need to be solved in solute transport modeling in porous earth media. The partial differential transport equation has been used in simulating solute transport in many models, such as MT3DMS (Zheng and Wang, 1999),

\[
\frac{\partial (\theta C)}{\partial t} = \frac{\partial}{\partial x_i} \left( \theta D_{ij} \frac{\partial C}{\partial x_j} \right) - \frac{\partial}{\partial x_i} (\theta v_i C) + q_s C_s 
\]  \hspace{1cm} (7)

where \( \theta \) is the porosity of the porous medium [dimensionless]; \( v_i \) is the seepage or linear pore water velocity [LT\(^{-1}\)], which related to the specific discharge or Darcy 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 sinks [ML\(^{-3}\)]; \( q_s \) is the volumetric flow rate per unit volume of aquifer representing fluid source (positive) and sink (negative) [T\(^{-1}\)].

The salinity or concentration obtained from equation above is used to calculate the water density for equation (2), (3) and (6). The variation of density is linear to salinity,

\[
\rho = \rho_f + Ra \cdot C 
\]  \hspace{1cm} (8)

where \( \rho \) is the density of salt water [ML\(^{-3}\)]; \( \rho_f \) is the density of fresh water [ML\(^{-3}\)]; \( Ra \) is the slope of the relationship between salt water density and fresh water density [dimensionless]; \( C \) is the solute concentration [ML\(^{-3}\)], the density from equation 8 is also applied in flow in conduits (equation 15).

2.3 Variable-density groundwater flow in karst conduits

Some numerical codes have been developed to simulate groundwater flow and solute transport in a karst aquifer, such as CAVE (Carbonate Aquifer Void Evolution) (Clemens et al., 1996; Liedl et al., 2003), MODFLOW-CFP (Shoemaker et al., 2008) and CFPv2 (Reimann et al., 2013). These codes have coupled pipe flow and porous media flow in the numerical model, but none of them is designed to simulate density-dependent seawater intrusion in a karst aquifer.
The Darcy-Weisbach equation is used to simulate groundwater flow in conduits, which is applicable to both laminar or turbulent flows (Shoemaker et al., 2008),

\[
\Delta h = h_L = f \frac{\Delta l V^2}{d^2 g}
\]  

where \( \Delta h \) or \( h_L \) is the head loss [L] measured along the pipe of length \( \Delta l \) [L]; \( f \) 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\(^{-1}\)].

The mean pipe flow velocity, \( V \), is equal to the volumetric flow, \( Q \) [L\(^3\)T\(^{-1}\)], divided by the cross-sectional area perpendicular to flow, \( A \) [L\(^2\)]. The Darcy-Weisbach equation can be reformulated to solve for volumetric flow rate, \( Q \) [L\(^3\)T\(^{-1}\)], rather than head loss \( \Delta h \), as followed,

\[
Q = A \sqrt{\frac{\Delta h d^2 g}{f \Delta l}}
\]

Bernoulli equation including head loss in the two sides of a conduit tube section could be written as:

\[
\frac{p_1}{\rho g} + z_1 + \frac{v_1^2}{2g} = \frac{p_2}{\rho g} + z_2 + \frac{v_2^2}{2g} + h_L
\]

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 two points [L]; \( v_1 \) and \( v_2 \) are the velocities [ML\(^{-1}\)] at the two points; \( h_L \) is the head loss [L] for water flow through the two points. The head loss term in Bernoulli equation:

\[
h_L = \frac{p_1 - p_2}{\rho g} + z_1 - z_2
\]

Rewrite equation 9 by the \( h_L \) in equation 11,

\[
Q = A \sqrt{\frac{\Delta h d^2 g}{f \Delta l}} = A \sqrt{\frac{2dg}{f} \left( \frac{1}{\rho g} \frac{dp}{dl} - \frac{dz}{dl} \right)}
\]

In order to derive the variable-density groundwater flow in the Darcy-Weisbach equation, the relationship of pressure term and equivalent freshwater head has been demonstrated by Guo and Langevin (2002) as,
\[ p = \rho_f g (h_f - z) \]  

Therefore, the relationship of flow rate respect to equivalent freshwater head and density could be presented by substituting the pressure differential term in equation 12 as follow,

\[ Q = A \sqrt{\frac{2dg}{f} \left( \frac{\rho_f}{\rho} \frac{dh_f}{dl} - \frac{\rho}{\rho} \frac{dz}{dl} \right)} \]  

Shoemaker et al. (2008) pointed out a linear relationship model for flow exchange between the conduit and porous media,

\[ Q_{n,ex} = \alpha_n \left( h_n - h_{i,k} \right) \]  

where \( Q_{n,ex} \) is the volume exchange of flow rate between the interface of conduit and matrix at conduit \( n \) \([L^3T^{-1}]\); \( h_n \) is the head at conduit node \( n \) \([L]\); \( h_{i,k} \) is the head at matrix cell \( i, k \) \([L]\); \( \alpha_n \) is the pipe conductance at conduit node \( n \) \([L^2T^{-1}]\).

The mass conservation of volumetric flow \( Q \) could be presented as follow,

\[ Q_n - Q_{n,ex} + Q_{n,R} = 0 \]  

where \( Q_n \) is the flow rate at conduit node \( n \) \([L^3T^{-1}]\); \( Q_{n,ex} \) is the volume exchange of flow rate between the interface of conduit and matrix at conduit node \( n \) \([L^3T^{-1}]\); \( Q_{n,R} \) is the direct conduit recharge at conduit node \( n \) \([L^3T^{-1}]\).

For most of the conduit nodes in this study, the node flow rate is:

\[ Q_n = Q_{n+1/2} + Q_{n-1/2} \]  

where \( Q_{n+1/2} \) is the volumetric flow rate between conduit node \( n \) and \( n+1 \) \([L^3T^{-1}]\), it can be calculated in equation 15.

While for the junction point, the node flow rate is different (Fig 2.1),

\[ Q_n = Q_{n+1/2} + Q_{n-1/2} + Q_{n+i-1/2} \text{ (junction)} \]  

where \( Q_{n+i-1/2} \) is the volumetric flow rate between conduit node \( n \) and \( n+i \) \([L^3T^{-1}]\).
2.4 Solute transport in karst conduits

Solute transport in the conduit is described by the one-dimensional advection equation as well, while mechanic dispersion within the conduit is ignored in the VDFST-CFP model in this study,

$$\frac{\partial C_i}{\partial t} = -q_i \frac{\partial C_i}{\partial x}$$ \hspace{1cm} (20)$$

where $C_i$ is the solute concentration [ML$^{-3}$] in conduit tube $l$; $q_i$ is the conduit flow velocity in conduit tube $l$, which could be calculated by $Q$ from the flow results within conduits.

Note there is no sink/source term for conduit transport equation. The flow exchange between conduit and matrix should be calculated by the equation as follow,

$$K_{n,ex} = \begin{cases} 
\left( \frac{Q_{n,ex}^+ C_{i,k}}{V_{i,k}} \right), & Q_{n,ex}^+ > 0 \\
\left( \frac{Q_{n,ex}^- C_{i,k}}{V_{i,k}} \right), & Q_{n,ex}^+ < 0 
\end{cases}$$ \hspace{1cm} (21)$$

where $K_{n,ex}$ is the advective exchange rate between a conduit node $n$ and respective matrix cell $i, k$ [ML$^{-3}$ T$^{-1}$]; $Q_{n,ex}^+$ is exchange flow rate [L$^3$ T$^{-1}$] at conduit node $n$ ($Q_{n,ex}^+ > 0$, flow direction is from matrix to conduit node; $Q_{n,ex}^+ < 0$, flow direction is from conduit node to matrix); $C_{i,k}$ is
the solute concentration of respective cell \( i, k \) in 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 respective cell \( i, k \) in porous medium at conduit node \( n \) [L\(^3\)].

For a single pipe, a weighted arithmetic mean of the concentration value \( C_n \) [ML\(^{-3}\)] at conduit node \( n \) is determined by the flow rate and concentration of neighboring conduit tubes, and exchanges with surrounding porous media (Spiessl et al., 2007),

\[
C_n = \frac{Q^+_{n-l/2}C_{n-l/2} + Q^+_{n+l/2}C_{n+l/2} + Q^+_{n,ex}C_{i,k} + \sum Q^+_{n,s}C_{n,s}}{Q^+_{n-l/2} + Q^+_{n+l/2} + Q^+_{n,ex} + \sum Q^+_{n,s}} \tag{22)
\]

where superscript \( f \) means either forward or backward direction of the conduit connected to node \( n \), the superscript \( + \) indicates the inflow terms at conduit node \( n \), which means that only inflow terms are used to compute the nodal concentration; \( C^f \) is the concentration of tube \( l \) connected to face \( f \) of the conduit node \( n \) [ML\(^{-3}\)]; \( C_{n,s} \) is the concentration of the source or sinks to the conduit node \( n \) [ML\(^{-3}\)]; \( Q^+_{n,l} \) is the discharge of tube \( l \) connected to face \( f \) into the respective conduit node \( n \) [L\(^3\)T\(^{-1}\)]; \( Q^+_{n,s} \) is the volumetric flow rate of a source term at conduit node \( n \) [L\(^3\)T\(^{-1}\)].

For multi-conduit, the concentration values at the junction point is (Fig 2.1),

\[
C_n = \frac{Q^+_{n-l/2}C_{n-l/2} + Q^+_{n+l/2}C_{n+l/2} + Q^+_{n-l/2}C_{n+l-1/2} + Q^+_{n,ex}C_{i,k} + \sum Q^+_{n,s}C_{n,s}}{Q^+_{n-l/2} + Q^+_{n+l/2} + Q^+_{n,ex} + \sum Q^+_{n,s}} \tag{23)
\]

where \( C_{n+l-1/2} \) is the solute concentration in the conduit between node \( n \) and node \( n+l \).

### 2.5 Roughness of conduits

The density-dependent Darcy-Weisbach equation (equation 14) is used in this study for modeling laminar and turbulent flow in karst conduits. The transition between laminar and turbulent flow is governed by the Reynolds number,

\[
Re = \frac{qd}{u} \tag{24)
\]
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 conduit diameter [L]; $u$ is the kinematic viscosity of the fluid [L$^2$T$^{-1}$].

Conduit walls are not totally smooth even in this idea model, surface roughness is a component of surface texture, which plays an important role in determining groundwater velocity in the conduit. For laminar flow, $f = Re / 64$, where $f$ is friction factor [dimensionless] (Reimann et al., 2011). For turbulent flow, the relationship between the friction factor, the Reynolds number, and the relative roughness is more complex, one model for this relationship is Colebrook-White Formula (Colebrook and White, 1937; Shoemaker et al., 2008).

$$
\frac{1}{\sqrt{f}} = -2\log \left( \frac{k_c}{3.71d} + \frac{2.51}{Re\sqrt{f}} \right)
$$

where $f$ is the friction factor [dimensionless]; $d$ is the conduit diameter [L]; $Re$ is the Reynolds number [dimensionless]; $k_c$ is the mean roughness height of the conduit wall micro-topography [L]. Mean roughness height $k_c$ is the key parameter to determine friction factor, it can be used as the height of micro-texture on the conduit wall. Therefore, for keeping the model reasonable and calculating convergence, the mean roughness height $k_c$ should be no more than 5 percent of conduit diameter.

Solving Colebrook-White Formula is not easy because it has to be solved in a numerical iteration. The Goudar-Sonnad equation (Goudar and Sonnad, 2008) is one of the approximations of the implicit Colebrook-White equation that is used in this paper. It is an accurate approximation to solve directly for the Darcy-Weisbach friction factor for a saturated circular pipe,

$$
\frac{1}{\sqrt{f}} = A \left[ \ln(C/Q) + D_{CFA} \right]
$$

where

$$
A = \frac{2}{\ln(10)}; \quad B = \frac{k_c}{3.71d}; \quad C = \frac{\ln(10)Re}{5.02}; \quad S = BC + \ln(C); \quad S = BC + \ln(C)
$$

$$
Q = S^{(x+1)}; \quad G = BC + \ln \frac{C}{Q}; \quad Z = \ln \frac{Q}{G}; \quad D_{LA} = Z \frac{G}{G+1};
$$

$$
D_{CFA} = D_{LA} \left( 1 + \frac{Z/2}{(G+1)^2 + (Z/3)(2G-1)} \right)
$$
Roughness is conceptualized by the high-frequency, short-wavelength and microstructures on the surface of pipe wall. However, for some situations such as caves on the conduit wall or collapse blocks on the conduit bottom in intensive-developed karst regions (Fig 2.2a), could not be identified as surface roughness. These large structures displayed above can be considered as pipe expansion and contraction (Fig 2.2b&c). Expansion and contraction interrupt the smooth flow of the fluid and generate additional head losses because of the flow separation and mixing they induce, this defined to be minor loss compare to the major loss, which is the regular head loss in the pipes due to frictional effects. For major loss, we can use Darcy-Weisbach equation; for minor loss, we express it in terms of loss coefficient (Cengel and Cimbaia, 2004).

\[
h_{\text{min}} = K_L \frac{V_j^2}{2g}
\]

\[
h_{\text{total}} = h_{\text{maj}} + h_{\text{min}} = \sum_i f \frac{L V_i^2}{d 2g} + \sum_j K_{L,j} \frac{V_j^2}{2g}
\]

where \(h_{\text{total}}\) is total head loss [L], \(h_{\text{maj}}\) is the major head loss [L], \(h_{\text{min}}\) is the minor head loss [L]; \(i\) represents each pipe section with constant diameter, \(j\) represents each component causes a minor loss; \(K_L\) and \(K_{L,j}\) are loss coefficient [dimensionless]; \(L\) pipe length [L]; \(d\) constant diameter [L]; \(V_i\) is the flow velocity of fluid flows in constant diameter section [LT\(^{-1}\)], \(V_j\) is the flow velocity of fluid flows into the component [LT\(^{-1}\)].

Loss coefficient calculations are given in below (Crane CO., 2009), we only consider the sudden expansion and contraction.

\[
K_{\text{exp}} = \frac{(1 - \beta_c^2)^3}{\beta_c^4}
\]

\[
K_{\text{con}} = \frac{0.5(1 - \beta_c^2)}{\beta_c^4}
\]
where $K_{\text{exp}}$ is the loss coefficient of expansion [dimensionless], $K_{\text{con}}$ is the loss coefficient of contraction [dimensionless]; $\beta_e$ and $\beta_c$ are the ratio of smaller diameter to larger diameter [dimensionless], for the expansion case, $\beta_e = D / D_e$; for the contraction case, $\beta_c = D_e / D$. Other types of loss coefficient can be found in relevant books (Crane CO., 2009; Vengel and Cimbaia, 2004; Menon, 2005; Roberson et al., 1998).

Based on the equation 29 and 30 above, the total head loss of conduit with an expansion which represents a cave on conduit wall or a contraction which represents stone stacked on the bottom of conduit is expressed below, for conduit with an expansion (Fig 2.2b):

$$V_1 \pi \left( \frac{D}{2} \right)^2 = V_2 \pi \left( \frac{D_e}{2} \right)^2 = V_3 \pi \left( \frac{D}{2} \right)^2$$  \hspace{1cm} (31)

$$V_1 = V_3, V_2 = \beta_e^2 V_1$$  \hspace{1cm} (32)
\[ h_{\text{total}} = \sum_i f \frac{L_i}{D_2} \frac{V_i^2}{2g} + \sum_j K_{i,j} \frac{V_j^2}{2g} \]
\[ = f \frac{L_1 + L_2}{D_2} \frac{V_1^2}{2g} + \frac{L_2}{D_2} \frac{V_2^2}{2g} + \frac{(1 - \beta_c^2)^2}{\beta_c^4} \frac{V_1^2}{2g} + \frac{0.5(1 - \beta_c^2)^2}{\beta_c^4} \frac{V_2^2}{2g} \]

where \( \beta_c \) is the ratio of diameters, \( \beta_c = D_c / D_e \).

for conduit with a contraction (Fig 2.2c):

\[ V_1 \pi \left( \frac{D}{2} \right)^2 = V_2 \pi \left( \frac{D}{2} \right)^2 = V_3 \pi \left( \frac{D}{2} \right)^2 \]

\[ V_1 = V_3, \quad V_2 = \left( \frac{1}{\beta_c^2} \right) V_1 \]

\[ h_{\text{total}} = \sum_i f \frac{L_i}{D_2} \frac{V_i^2}{2g} + \sum_j K_{i,j} \frac{V_j^2}{2g} \]
\[ = f \frac{L_1 + L_3}{D_2} \frac{V_1^2}{2g} + \frac{L_2}{D_2} \frac{V_2^2}{2g} + \frac{0.5(1 - \beta_c^2)^2}{\beta_c^4} \frac{V_1^2}{2g} + \frac{(1 - \beta_c^2)^2}{\beta_c^4} \frac{V_2^2}{2g} \]

where \( \beta_c \) is the ratio of diameters, \( \beta_c = D_c / D_e \).

Minor loss parts can be expressed in terms of equivalent length \( L_{eq} \) (Vengel and Cimbaia, 2004), for conduit with an expansion (Fig 2.2b):

\[ f \frac{L_2}{D_2} \frac{V_2^2}{2g} + \frac{(1 - \beta_c^2)^2}{\beta_c^4} \frac{V_2^2}{2g} + \frac{0.5(1 - \beta_c^2)^2}{\beta_c^4} \frac{V_1^2}{2g} = f \frac{L_{eq}}{D} \frac{V_1^2}{2g} \]
\[ \Rightarrow L_{eq} = L_2 \beta_c^5 + \frac{D(1 - \beta_c^2)^2}{f \beta_c^4} + \frac{D(1 - \beta_c^2)^2}{2f} \]

for conduit with a contraction (Fig 2.2c):

\[ f \frac{L_2}{D_2} \frac{V_2^2}{2g} + \frac{0.5(1 - \beta_c^2)^2}{\beta_c^4} \frac{V_2^2}{2g} + \frac{(1 - \beta_c^2)^2}{\beta_c^4} \frac{V_2^2}{2g} = f \frac{L_{eq}}{D} \frac{V_1^2}{2g} \]
\[ \Rightarrow L_{eq} = \frac{L_2}{\beta_c^3} + \frac{D(1 - \beta_c^2)^2}{2f \beta_c^4} + \frac{D(1 - \beta_c^2)^2}{f \beta_c^8} \]

and the total loss equation of expansion and contraction by using equivalent length is,
\[ h_{\text{total}} = f \frac{L_1 + L_2 + L_{eq}}{D} \frac{V_1^2}{2g} \]  

For large size reduction, the loss coefficient of reducer/expander is very high which can cause an unacceptable pressure drop in such cases. Therefore, it is recommended that the expansion and reduction are less than 30 percent of diameter.
CHAPTER THREE
NUMERICAL MODEL SETUP

3.1 Conceptual model

Fig 3.1 shows the conceptual model of this study which represents the seawater intrusion in most coastal karst aquifers. Seawater intrudes inland in two ways, one is the gradual transport and dispersion in porous media, leading to fresh-salt water mixing zone at the interaction of seabed and continental shelf. In the other way, seawater backflows into submarine karst conduits when hydraulic gradient is landward, and contaminates further inland freshwater.

Two synthetic numerical models have been designed as benchmarks to validate the VDFST-CFP model. The horizontal case is used to verify the groundwater flowing and solute transporting in discrete-continuum approach; the vertical case is developed to test the performance of density-dependent flow and transport (Xu and Hu, 2017a). In this study, we mainly focus on the vertical case, the model is established based on the Upper Florida Aquifer in the WKP (Woodville Karst Plain) which the average elevation of conduit system is 285 BSL (Davis et al., 2010; Davis and Verdi, 2014; Kincaid et al., 2005; Kincaid and Werner, 2008; Xu and Hu, 2017a).

3.2 Model domain

It is obvious that the real karst aquifer cannot be modeled exactly in any numerical model, the extremely large number of discretization grid for real space size is unaffordable for numerical
computing, a 2D vertical benchmark shown in Fig.5 can be regarded as a much smaller spatial scale of the WKP theoretical model.

Fig 3.2 Schematic finite difference grid discretization and boundary conditions applied in the vertical benchmark case. 
- Light blue represents porous media; 
- Green represents conduit system; 
- Dark blue represents sea water boundary, the constant head is 0.0 ft and constant concentration is 35.0 PSU at sea water boundary; 
- Yellow represents fresh water boundary, where constant head is 5.0 ft and constant concentration is 0.0 PSU.
The spatial discretization of this aquifer system consists of 1 row, 70 columns and 35 layers. The rows and columns width of each cell is 50 ft by 50 ft, the thickness of each layer is 10 ft. The elevation of surface layer starts from 34 ft BSL (Below Sea Level) at the left and gradually rises to 19 ft BSL at the right, which is simulated as a confined aquifer. In single conduit model, the conduit system starts from the top of column 11#, downward to the layer 29#, and then extends horizontally to the column 68#, finally upward to the top of column 68# (Fig 3.2a). In multi-conduit model, another conduit is added on the single conduit model which starts from row 18#, column 12# horizontally extends to column 34#, and then downward to connect with main conduit (Fig 3.2b). In the dual-conduit model, another conduit is added on the single conduit model which starts from row 26#, column 12#, and then horizontally extends to connect with main conduit at column 68# (Fig 3.2c). In both models, the first and last node of conduit system is set as submarine spring and inland karst spring respectively.

3.3 Boundary conditions and initial conditions

No flow boundary is applied on the top and bottom of this model. The freshwater boundary on the rightmost column is constant head boundary which is 5.0 ft and constant salinity is 0 PSU; the seawater boundary on the leftmost column is set as 0.0 ft constant head and 35.0 PSU constant concentration (Fig 3.2).

The initial condition of hydraulic head in porous media gradually rises from 0.0 ft at the leftmost column to 5.0 at rightmost column, the vertical gradient in each layer is zero. The salinity in porous media is set to be 0.0 at the beginning except the boundary condition. The initial conditions of conduit system are the same as those in the surrounding porous media. In the VDFST-CFP, a rigorous convergence criterion for both porous media and conduits is needed, therefore, the time step size is specified as 0.0005 day and the total computation time is 0.2 day.

3.4 Hydraulic properties

Davis et al. (2010) proposed and calibrated most of parameter values are assigned to this theoretical model, which are based on the data collection from Upper Floridan Aquifer in the WKP. For the high-resolution requirement of vertical discretization in variable-density numerical modeling, the conduit diameter is set to be as small as 0.8 ft, the mean roughness height is 0.008 ft. Hydraulic conductivity in porous media and conduit-matrix exchange permeability are 7500 ft/day, porosity is 0.003, specific storage and dispersivity are 0.00005 and 32.8 ft respectively.
Table 4.1 Parameter values of the conduit system and porous media in the VDFST-CFP model

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Porous media</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Conductivity</td>
<td>7500</td>
<td>ft/day</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.003</td>
<td>dimensionless</td>
</tr>
<tr>
<td>Specific storage</td>
<td>0.00005</td>
<td>dimensionless</td>
</tr>
<tr>
<td>Dispersivity</td>
<td>32.8</td>
<td>ft</td>
</tr>
<tr>
<td>Conduit system</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Diameter</td>
<td>0.8</td>
<td>ft</td>
</tr>
<tr>
<td>Mean roughness height</td>
<td>0.008</td>
<td>ft</td>
</tr>
</tbody>
</table>

3.5 Simulation results

(a) Seawater intrusion in single-pipe model

(b) Seawater intrusion in one-pipe-and-half-pipe model

Fig 3.3 Salinity simulation in VDFST-CFP model. (a) is seawater intrusion in single-pipe model; (b) is seawater intrusion in multi-pipe model; (c) is seawater intrusion in double-pipe model. Yellow represents high concentration, blue represents low concentration.
Fig 3.3 shows seawater intrusion of VDFST-CFP method in single-pipe model, one-pipe-and-half-pipe and double-pipe model. Saltwater front moves further landward in conduit than in porous media, three models have a roughly same intrusion speed along conduit. The salinity concentration in conduit system is heavily influenced by the surrounding matrix blocks, and influences the whole salinity distribution in matrix domain, this influence effects of double-pipe model and multi-pipe model to a higher degree than single-pipe model.

### 3.6 Parameter sensitivity study

Parameter sensitivity study has been applied in this paper to investigate the effect of parameter variation on the seawater intrude distance both in conduit and porous media. The evaluated factors are the number of components, conductivity, diameter, dispersivity, exchange interaction, porosity, mean roughness height and specific storage. Among them, one pair of components contains one expansion and one extraction, both with a component length of 2.5ft and diameter difference of 0.2ft. The results of parameter effect are showed in Fig 3.4, the position of mixing zone in matrix is defined as the east-most column number in layer #20 with salinity larger than 10.0 PSU, the position of mixing zone in conduit is defined as the column number of the east-most conduit node with salinity larger than 10.0 PSU. Only single-pipe model is considered in this investigation, double-pipe model and multi-pipe model should display a similar trend.
The effect of parameters variation on seawater intrusion, the plots on the left column are the simulations in the conduit, the plots on the right column are the simulations in the matrix (layer #20).
The variations of parameters such as dispersivity, exchange interaction between conduit and matrix, and specific storage don’t arouse an obvious change on seawater intrusion either in conduit or matrix, these parameters appear to be unimportant to the simulation. The number of components plays a role on seawater intrusion in conduit system, seawater intrudes backward with more components, while the variation of components number changes little on seawater intrusion in matrix. The mean roughness height plays a smaller role on simulations relative to macro-structures but with a similar pattern. The variations of conductivity, diameter and porosity significantly affect the position of mixing zone in both conduit system and porous media. Saltwater moves more landward in conduit and matrix due to higher velocity in larger diameter conduit, this result is similar with Xu and Hu (2017a). In a similar mode, larger conductivity leads to further landward of seawater intrusion, the salinity plume tends to spread broadly and quickly with large matrix conductivity. Porosity is another important parameter, seawater intrusion in conduit is not
independent with matrix porosity, higher porosity results in backward saltwater movement. On the other hand, smaller porosity causes less advection and dispersion in solute transporting from conduit system to porous media, thus the mixing zone in matrix is strongly influenced by seawater moving in conduit, for this reason of lower porosity allows further landward movement of seawater intrusion in porous media. However, the effect of porosity variation on seawater intrusion in conduit of vertical case is different from the sensitivity analysis of horizontal case (Xu and Hu, 2017a).

The parameter sensitivity study provides a direct perspective of how the parameters influence the seawater intrusion, and an instruction of model calibration (calibration is not considered in this study since the current model is just for synthetic case). However, for exact investigating the importance of different parameters, further sensitivity analysis has to be conducted.
CHAPTER FOUR
SENSITIVITY ANALYSIS

Sensitivity analysis is used to investigate whether a certain percentage change in a parameter has any significance on final results, that is whether it is a dominant parameter (Bear et al., 1992). In this study, seven parameters (conductivity, conduit diameter, exchange permeability between conduit and matrix, porosity, mean roughness of conduit wall, specific storage and dispersivity) are evaluated by local sensitivity analysis and global sensitivity analysis. Sensitivity analysis of macro-structures is not considered for the reason that there are three parameters that determine each component and the number of component cannot be evaluated by local or global analysis. Only single conduit model is calculated in this study, multiple conduit models are not included since they exhibit similar pattern.

4.1 Methodology

4.1.1 Local sensitivity analysis

In this study, the forward difference approximation is used to calculate sensitivity of \( i \)th observation with respect to \( j \)th parameter (Hill and Tiedeman, 2006):

\[
\left( \frac{\partial y'_i}{\partial b_j} \right)_{b} \approx \frac{y'_i(b + \Delta b) - y'_i(b)}{\Delta b_j}
\]

where \( y'_i \) is the result of \( i \)th observation; \( b_j \) is the \( j \)th estimated parameter; \( b \) is the vector of parameter values; \( \Delta b \) is a vector of zero except that the \( j \)th parameter equals \( \Delta b_j \), \( \Delta b_j \) should be 1 to 5 percent of \( b_j \) (Saltelli et al., 2000).

Different parameters have different units, for making comparability between different parameters available, sensitivities are converted to dimensionless scaled form (Hill, 1992; Hill et al., 1998):

\[
dss_{ij} = \left( \frac{\partial y'_i}{\partial b_j} \right)_{b} \left| b_j \right|
\]

where \( dss_{ij} \) is dimensionless scaled sensitivity of \( i \)th observation respect to \( j \)th parameter.
The total effect of different observations for one parameter is reflected in composite scaled
sensitivity. It is calculated by following equation (Hill, 1992; Anderman et al., 1996; Hill et al.,
1998):

\[
\text{css}_j = \sum_{i=1}^{N} \left( \frac{dss_{ij}^2}{N} \right)^{1/2}
\]  

(42)

where \( css_j \) is composite scaled sensitivity of \( j \)th parameter; \( N \) is the number of observations.

4.1.2 Global sensitivity analysis with Morris Method

Variations of some parameters, such as conduit diameter and mean roughness height, may
influence each other on the estimation. Global sensitivity analysis fully considered the significance
of one parameter under interactions with other parameters. In this study, the Morris method
(Morris, 1991; Saltelli et al., 2004) is applied to evaluate the global sensitivities of parameters.
Morris method is one-at-a-time experiment, it is based on element effect which is the effect of
changing one parameter at a time. The trajectory sampling is used in Morris method, to compute
\( k \) parameters, \((k+1)\) simulations are calculated with a random start sampling point in one trajectory,
input space of each parameter is discretized into \( p \) levels and the whole calculation contains \( r \)
trajectories. The element effect of changing \( i \)th parameter in \( j \)th trajectory is:

\[
d_{ij} = \frac{y(x_j + e_i \Delta) - y(x_j)}{\Delta}
\]  

(43)

where \( x_j = (x_1, x_2, ..., x_k) \) of \( j \)th trajectory; \( \Delta = 1/(p-1) \); \( e_i \) is a vector of zeros but with a
unit as its \( i \)th component.

Once computations are completed, the average \( (u) \) of one parameter in \( r \) trajectories reflects
an estimation of total-order effect, and standard deviation \( (\sigma) \) describes variability of parameter
space and extent to parameter interactions (Herman et al., 2013).

\[
u_i = \frac{1}{r} \sum_{j=1}^{r} d_{ij}
\]  

(44)

\[
\sigma_i = \sqrt{\frac{1}{r} \sum_{j=1}^{r} (d_{ij} - u_i)^2}
\]  

(45)
The specified value in local analysis and estimation ranges in global analysis of seven parameters are listed in Table 4.2.

Table 4.2 The specified values of local analysis and value ranges of global analysis of seven parameters, the parameters are cited from Xu et al. (2017a) and Davis et al. (2010)

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Specified value</th>
<th>Estimation range</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conductivity</td>
<td>7500</td>
<td>4500 ~ 10500</td>
<td>ft/day</td>
</tr>
<tr>
<td>Diameter</td>
<td>0.8</td>
<td>0.48 ~ 1.12</td>
<td>ft</td>
</tr>
<tr>
<td>Dispersivity</td>
<td>32.8</td>
<td>19.68 ~ 45.92</td>
<td>ft</td>
</tr>
<tr>
<td>Exchange permeability</td>
<td>7500</td>
<td>4500 ~ 10500</td>
<td>ft/day</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.003</td>
<td>0.0018 ~ 0.0042</td>
<td>dimensionless</td>
</tr>
<tr>
<td>Mean roughness height</td>
<td>0.008</td>
<td>0.0048 ~ 0.0112</td>
<td>ft</td>
</tr>
<tr>
<td>Specific storage</td>
<td>5.00e-5</td>
<td>3.00e-5 ~ 7.00e-5</td>
<td>dimensionless</td>
</tr>
</tbody>
</table>

4.2 Local sensitivity analysis

The salinity CSS (composite scaled sensitivity, equation 42) and hydraulic head CSS are calculated in porous media and conduit for each parameter, the specified values are listed in Table.1. The sensitivities of conduit is calculated from column #15, which is close to submarine spring, to column #65, which is near fresh water spring. The sensitivities of porous media is starting from column #15 to column #65 in layer #20, which is 9 layers above the conduit and located at the center of domain. In general, larger CSS value represents more significance of such parameter to simulation.

The results of local sensitivity analysis in conduit are showed in Fig 4.1, which are correspond with the results in section 3.6 in general. The salinity is more sensitive to changes of parameters than hydraulic head, diameter is the most important parameter to conduit simulations due to largest CSS values, because diameter directly determines the flow velocity in conduit system (Fig 4.1). Porosity also play an important role in the simulation, the possible reason is the interaction between matrix blocks near the conduit and conduit system is significant influenced by porosity. Range of column#40 to #45 shows the highest CSS values of all parameters along conduit, which reflects a rough location of salt-fresh water mixing zone of all simulations.
Fig 4.1 CSS values in conduit. Upper plot is the total, salinity and head CSS values of seven parameters to conduit simulation; lower plot is the total CSS values at different locations along conduit.

Fig 4.2 shows composite scaled sensitivity in layer #20 of seven parameters, the whole matrix domain should exhibit the same pattern. CSS values in matrix is much smaller than conduit, due to the matrix domain is two-dimension and dispersion is fully considered in it. In porous media, the simulation results are more sensitive to porosity and conductivity than diameter, since porosity and conductivity are matrix properties, and diameter only strong influence the matrix elements near the conduit system. Dispersivity is also critical to the simulation when compared with other non-dominant parameters, this point isn’t showed in the results of section 3.6. The largest CSS values in layer #20 is located from column #24 to #29, which means the position of mixing zone.
4.3 Global sensitivity analysis

Global sensitivity analysis provides a better understanding and perspective of parameter sensitivities on seawater intrusion model. Morris trajectory method is applied for reducing computational cost, a simulation with level $p=4$ and path $r=10$ is good enough for most cases (Saltelli et al., 2004). According to results of local analysis, the evaluation positions of global analysis are accordance with the location of largest CSS values, which is column 43 in the conduit and column 26 in the porous medium. Therefore, Morris trajectory sampling method analysis with four level and ten paths is implemented and the results are listed in Fig 4.3.
Fig 4.3 Mean and standard deviation of element effect of each parameter: (a) salinity in the conduit; (b) head in the conduit; (c) salinity in the matrix; (d) head in the matrix.
The results of global sensitivity analysis reflect a pattern similar to the local analysis. The mean and standard deviation to salinity simulation is much larger than head simulation, and the values to conduit simulation is much larger than matrix simulation. Porosity, diameter and conductivity are the top three on the values of mean and standard deviation, which indicates they are important parameters in both conduit and matrix, also in both head simulations and salinity simulations. In the results of conduit simulation (Fig 4.3a&b), diameter is the most important parameter since it directly affects the flow velocity; the effect of conductivity and porosity are nearly same to the head and salinity simulation in the conduit, which seems different from local analysis (Fig 4.1). The mean and variance of specific storage is nearly zero, it can be concluded that the conduit simulation is independent of specific storage; the mean values of roughness is a bit larger than specific storage since it has a mild effect on the conduit flow velocity. To the results of matrix simulation (Fig 4.3c&d), porosity is the most important coefficient; mean value of diameter is larger than conductivity to salinity simulation while smaller than conductivity in head simulation, which illustrated the groundwater simulation of conduit system major influences the salinity distribution in matrix due to saltwater exchanging between them. Element effect of roughness in matrix simulation is nearly zero since the evaluation location is far away from conduit system.

**4.4 Discussion of sensitivity analysis**

The parameters in the previous sensitivity analysis are calibrated in the numerical modeling of Woodville Karst Plain (Xu et al., 2017a; Davis et al., 2010). While the specific value and value
range of these parameters are not reasonable for the most of karst aquifer, especially large conductivity with a small porosity. In this discussion, some value are adjusted and recalculated in the sensitivity analysis. The new parameters are listed in Table 4.3.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Specified value</th>
<th>Estimation range</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conductivity</td>
<td>750</td>
<td>600 ~ 900</td>
<td>ft/day</td>
</tr>
<tr>
<td>Diameter</td>
<td>0.8</td>
<td>0.64 ~ 0.96</td>
<td>ft</td>
</tr>
<tr>
<td>Dispersivity</td>
<td>32.8</td>
<td>26.24 ~ 39.36</td>
<td>ft</td>
</tr>
<tr>
<td>Exchange permeability</td>
<td>750</td>
<td>600 ~ 900</td>
<td>ft/day</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.003</td>
<td>0.024 ~ 0.036</td>
<td>dimensionless</td>
</tr>
<tr>
<td>Mean roughness height</td>
<td>0.008</td>
<td>0.0064 ~ 0.0096</td>
<td>ft</td>
</tr>
<tr>
<td>Specific storage</td>
<td>5.00e-3</td>
<td>4.00e-3 ~ 6.00e-3</td>
<td>dimensionless</td>
</tr>
</tbody>
</table>

The results of new sensitivity analysis (Fig 4.4 & Fig 4.5) is different from the previous calculation, the diameter is the most important parameter in the conduit simulation and matrix simulation. Some unimportant parameter such as specific storage, dispersivity become more important in this simulation. The largest CSS value along the conduit is located at Column 19 which is also the mixing position of freshwater and seawater, the seawater intrusion in conduit system and porous media is more sensitive to conductivity and specific storage than porosity. The CSS value along the Layer 20 has two peaks, one is Column 7 which is the mixing position, the parameters of porous media get the highest value at here; another is Column 11 which contains the vertical part of conduit system, the parameters of conduit get the highest value at Column 11. The global analysis is conducted at Column 19 in the conduit system, and Column 7 in the Layer 20 which mainly measure the sensitivities of parameters of porous media. The element effect of conduit diameter in the matrix global analysis is much lower relative to the results of local analysis, because Column 7 in the Layer 20 is not sensitive to the parameters of conduit system.

The new sensitive analysis measured the importance degree of each parameters for the normal karst aquifer, the results also reflect a more convincing value of sensitivities: conductivity should be more important than porosity in solute transport and head distribution, the dispersion coefficient is also a major factor in salinity distribution.
Fig 4.4 Results of new local sensitivity analysis: (a) total, salinity and head CSS values of seven parameters to conduit simulation; (b) total CSS values at different locations along conduit; (c) total, salinity and head CSS values of seven parameters to matrix simulation (Layer 20); (d) total CSS values at different locations along Layer 20.
Fig 4.4 Continued.

Fig 4.5 Mean and standard deviation of element effect of each parameter in new global sensitivity analysis: (a) salinity in the conduit; (b) head in the conduit; (c) salinity in the matrix; (d) head in the matrix.
Fig 4.5 Continued.
CHAPTER FIVE

SCENARIOS STUDY

Xu et al. (2017b) indicated the salinity and sea level at the submarine spring are the most important boundary conditions in the head and salinity simulations of dual-permeability system. For evaluating the effect of boundary conditions on seawater intrusion in VDFST-CFP model, salinity variation and sea level variation at the submarine spring vent are simulated and quantitatively measured in this chapter. Only single-pipe model is considered in this investigation, double-pipe model should display a similar trend.

5.1 Salinity variation at the submarine spring

Salinity at the submarine spring varies due to precipitation and freshwater discharge producing dilution of salt water. In a high precipitation period, rainfall recharge and freshwater discharge dilute the seawater at submarine spring; while in the low rainfall period, the high concentration seawater flows into the submarine spring, the seawater intrusion under maximum salinity is displayed in Fig.6. In order to investigate the impacts of salinity variation on seawater intrusion, four scenarios with different salinity (0.0 PSU, 10.0 PSU, 20.0 PSU, 30.0 PSU) at submarine spring are implemented with 0.0 m sea level. The results are showed in Fig 5.1.

Fig 5.1 shows that rainfall recharge and freshwater discharge strongly influence the seawater intrusion in conduit system, lower precipitation and freshwater discharge (higher salinity at submarine spring) move the salt/fresh mixing zone significantly landward. Alternatively, the salinity in the conduit system is also influenced by the precipitation and freshwater discharge, lower precipitation and freshwater discharge causes higher salinity in the conduit system. The shape of mixing interface in matrix influenced by the saltwater in the conduit and move backward slightly due to decreasing salinity at submarine spring. The comparison of four scenarios on seawater intrusion distance and salinity is showed in Fig 5.2, the seawater intrusion in the conduit system and porous media moves seaward average 7 cells and 1 cell, respectively, with 10 PSU decreasing at the submarine spring.
Fig 5.1 Salinity distribution under different salinity conditions at submarine spring which indicates various precipitation and freshwater discharge: from top to bottom, they are 0.0 PSU, 10.0 PSU, 20.0 PSU, 30.0 PSU at the submarine spring.
5.2 Sea level variation

Sea level is another important parameter that can impact the seawater intrusion, the variation of hydraulic head at the submarine spring and seawater boundary may change the whole hydraulic gradient in the conduit system and porous media. Four cases, -1.0 ft to 1.0 ft variation in sea level conditions at both sea boundary and submarine spring are considered in this study, while the salinity at the submarine spring and sea boundary remains 35.0 PSU. The simulations prove that the rise in sea level leads to a more severe seawater intrusion (Xu et al, 2017b) both in conduits and porous media (Fig 5.3). Fig 5.4 shows the comparison between intrusion distance in conduit and matrix under different sea level conditions. With the rising sea level, the variation of landward intrusion in conduit system is much more obvious than in porous media, which also indicates coastal karst aquifers are much more vulnerable than normal coastal aquifers to sea level variation since the karst conduit acts as the major pathway for seawater intrusion.
Fig 5.3 Salinity distribution under different sea levels: from top to bottom, they are -1.0 ft, -0.5 ft, 0.5 ft, 1.0 ft, the result of 0.0 ft is displayed in Fig 3.3(a).
Fig 5.4 Position of mixing zone in the matrix and conduit under various sea level, position of mixing zone is the rightmost cell which salinity is larger than 10 PSU in the Fig 5.3.
CHAPTER SIX
CONCLUSION

VDFST-CFP is a numerical method for modeling variable-density flow in a dual-permeability domain, especially for seawater intrusion in a coastal karst aquifer. In Chapter 2 and 3, the primary VDFST-CFP model (Xu and Hu, 2017a) is improved to account for multi-conduit system. The modified node flow and concentration equations are applied on the junction point of the conduit system. Currently, the multi-conduit system model only utilizes two pipes since the computation burden become much larger even only one pipe is added. The simulation results show that the seawater plumes in the porous media are larger in the dual-conduit system, which may causes more serious environmental problems. According to this result, the environmental status of real coastal karst aquifer is even worse due to much more complex and wider distributed conduit system. Another newly developed modification is the conduit wall roughness. The size of micro-structure on conduit wall is considered as mean roughness height, and implemented in Goudar-Sonnad equation (Goudar and Sonnad, 2008), the parameter sensitivity study indicates the larger mean roughness height results in relatively slower conduit flow. On the other hand, the large structures on conduit wall are considered as contraction and expansion in pipe flow, these components may cause additional minor head loss due to energy consuming at the location of flow change, which is considered as equivalent pipe length. The parameter sensitivity study shows that more components of macro-structures lead to obviously slower seawater intrusion in conduit while plays little effect on matrix simulation. In the most numerical simulation of karst aquifers, the large components on conduit wall are seldom to be considered, or just be regarded as a part of a sinuosity factor. This study reveals the significant effect of large components and provides a mathematic method to take into account them in the flow of karst conduit system.

In Chapter 4, A sensitivity study conducted in a vertical case included local analysis and global analysis. Sensitivity analysis shows that conduit diameter, conductivity and porosity are top three important parameters both in conduit and matrix. The salinity simulation is more sensitive to the variation of parameters relative to the head simulation, similarly the conduit simulation is more sensitive compared with matrix simulation. In the conduit system, diameter is the most important parameter since it directly influences the flow velocity; while in the matrix, porosity has the largest
CSS value and element effect, because it determines the concentration distribution in the porous media.

In Chapter 5, the impact of salinity variation at a submarine spring and sea level variation on the seawater intrusion is analyzed in this study. Salinity at submarine spring is diluted by the precipitation and freshwater recharge causing a seaward seawater migration. In addition, the sea level rise moves the seawater intrusion further landward, the interface met even reach the vertical part of conduit system under sea level of 1.0 ft. In general, seawater intrusion in both conduit system and matrix are influenced by the salinity at the submarine spring and sea elevation, while the intrusion in conduit is more sensitive to the change of boundary conditions.

As Xu and Hu (2017a) demonstrated, the Newton-Raphson method strongly controls the model accuracy and mass balance in conduit flow, smaller conduit diameter produce higher numerical stability. Truncation errors may be non-neglectable for solving advection-dominated solute transport in the matrix near conduit system. The accuracy of the vertical model in this paper is not improved, especially the double-conduit model may cause unacceptable mass balance when diameter is set too large, such as 1.5 ft. For reducing the computation time, author tried to change the layer thick from 10 ft to 15 ft, but the results showed large errors in salinity distribution at bifurcation point. Future studies should continue investigating how to improve simulation accuracy, reduce computation burden and expand the application, GPU-accelerated computing or MPI calculation may be an effective method.
REFERENCES


Goudar C.T. and Sonnad J.R. (2008). Comparison of the iterative approximations of the Colebrook-White equation: Here’s a review of other formulas and a mathematically exact formulation that is valid over the entire range of Re values. Hydrocarbon processing: 87 (8).


BIOGRAPHICAL SKETCH

Zhongyuan Xu

Education

08/2015-present  Graduate study of master program in Geology
Study area is Hydrogeology/Groundwater modeling
Department of Earth, Ocean & Atmospheric Science
Florida State University (FSU), FL, United State
Supervisor: Dr. Bill X. Hu

09/2011-06/2014  Master of Engineering in Geological Engineering
School of Environment and Civil Engineering
Chengdu University of Technology (CDUT), Chengdu, China
Supervisor: Dr. Tianbin Li

09/2007-06/2011  Bachelor of Engineering in Prospecting Techniques and Engineering
School of Environment and Civil Engineering
Chengdu University of Technology (CDUT), Chengdu, China

Research knowledge and interests

1. Numerical simulation of variable-density flow and solute transport in porous media, fracture media and karst conduit area.
2. Sensitivity and risk analysis of numerical models and hydrologic parameters.
3. Surface water and groundwater interaction coupled model.
4. Regional hydrogeological survey, engineering geological survey.
5. Hydrological laboratory tests, soil and rock laboratory tests.
6. Numerical simulation on failure mechanics of rock and rock behavior under hydro-mechanical or thermal-mechanical coupling effect.

Research experience

12/2015-present  Numerical modeling of seawater intrusion in coastal karst aquifer with well-developed conduits: A development of VDFST-CFP (Variable
Density Flow and Solute Transport - Conduit Flow Process) model (Host: Dr. Bill X. Hu)

09/2015-present Laboratory experiment of conduit flow in Woodville Karst Plain (Host: Dr. Stephen Kish)

10/2013-06/2014 Project of National Natural Science Foundation of China (NO. 41230635): The mechanism analysis and prediction of rock burst in the deep and large tunnels under multi-field couplings (Host: Dr. Tianbin Li)

08/2012-03/2014 Open fund project of State Key Laboratory of Geohazard Prevention and Geoenvironment Protection (NO. SKLGP2011K008): Mechanical behavior and microscopic mechanism of heterogeneous soft rock (Host: Dr. Liangxiao Xiong)

09/2012-12/2012 Numerical simulation approach to geostatic stress measurements of the tunnel in the mountain Zhegu (Host: Dr. Tianbin Li)

09/2011-04/2012 Centrifuge physical modeling of large-scale slope slide in Panzhihua Airport (Host: Dr. Tianbin Li)

11/2010-06/2011 Karst hydrological study of Xu-Gu Expressway (Host: Dr. Huijun Liu)

Academic skills
Compiling Skills: Fortran, MATLAB
Codes: MODFLOW, MT3DMS, MODFLOW-CFP, SEAWAT
Software: AutoCAD, ArcGIS, Origin, Adobe Illustrator, Particle Flow Code, FLAC3D, ANSYS

Publications

Zhongyuan Xu, Tianbin Li, Guoqing Chen, Chunchi Ma, Shili Qiu and Zhi Li (2016). The Grain-Based Model Numerical Simulation of Unconfined Compressive Strength Experiment Under Thermal-Mechanical Coupling Effect. KSCE, under review.


**Honors and awards**

Awarded for Excellent Graduate Students by CDUT, 12/2012

Awarded the 2nd Class Scholarship for the Excellent Graduates by CDUT, 12/2012

Awarded a scholarship by the National Scholarship for Outstanding Graduate Students, 11/2012

Awarded the School Excellent Social Worker by CDUT, 11/2008