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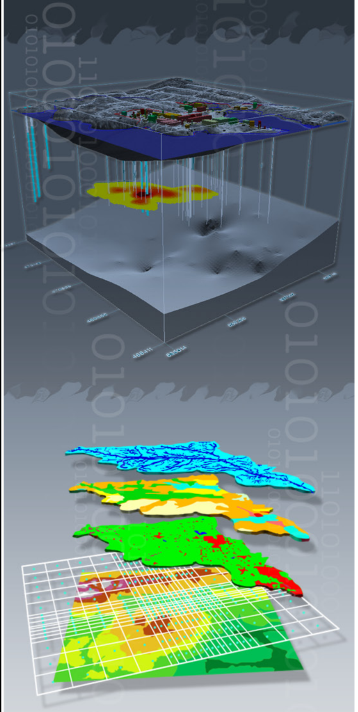

Abstracts of Papers & Presentations of MODFLOW-SURFACT™ and MODHMS®

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Bedekar, V., S. Panday, H. Ahn, and F. Miralles-Wilhelm, 2006. **Surface-water Groundwater Interaction Model for Marsh Driven Operations to Manage the Ecosystem of the Rocky Glades,** *MODFLOW and More 2006 Managing Groundwater Systems – Conference, Golden, CO., 2006.*

The L-31N canal cuts through the Rocky Glades of eastern Everglades National Park (ENP) in South Florida. Low stages in the L-31N canal cause drainage of the adjacent wetlands of the ENP leading to upland species invasion and increased fire risk. The South Florida Ecosystem Office of the National Park Service (NPS) is developing a Marsh Driven Operations Plan (MDOP), which seeks to minimize this drainage by pumping water from the L-31N canal into detention areas west of the L-31N canal to maintain water levels such that the west-to-east gradient draining the Rocky Glades is reduced. Water levels in these detention areas need to be well managed since high levels may cause the adjacent wetlands to be excessively flooded by water of high phosphorous concentrations from the L-31N canal; which is also detrimental to the wetlands. To analyze the operations of the MDOP for pumps and detention basins, a modeling investigation was conducted using MODHMS©, a surface-water groundwater interaction model. The model was calibrated and verified against flow, stage and water-level data over a period of three years from January 1, 2000 through December 31, 2002. The MDOP operations were then investigated for effectiveness. Model development and results are discussed.

Beeson, P, Duffy, C, Springer, E, Panday, S. (2004). **Integrated Hydrologic Models for Closing the Water Budget: Whitewater River Basin, Kansas,** *Eos Trans. AGU, 85(47), Fall Meet. Suppl., Abstract H34B-05.*

Groundwater and its recharge are unobserved and unmeasured components of the water cycle of a river basin. The objectives of this study were: 1) to evaluate the groundwater component of the water balance for the Whitewater River Basin using a 3-D saturated groundwater model, 2) to compare the groundwater model results with a fully integrated hydrologic model and, 3) to describe the spectral frequency response of the basin to long-term climate forcing. The basin is the Whitewater River, near Wichita, Kansas. The basin has an area of 1,100 square-kilometers, an elevation range of 380 - 470m (amsl), and an average annual precipitation of 858 millimeters. The near-surface geology is comprised of a weathered shale overlying limestone bedrock of Mississippian age. Streamflow and weather records are available from 1960. A steady-state saturated groundwater model (MODFLOW) was implemented assuming a simple two-layer conceptual model. A total of 422 wells with static water levels were available. Using a subset of the wells, a steady-state calibration of MODFLOW was performed by adjusting permeability between the two layers. Steady-state calibration resulted in an R2 of 0.89 for predicted and observed water levels. The remaining wells were used for validation, with an R2 of 0.92. The next step constructed the transient model using a fixed percentage of rainfall as groundwater recharge. For a single observation well the R2 was 0.89 (observed vs. predicted) for the transient calibration and 0.77 for the validation for a year simulation. The final step was to compare MODFLOW to an integrated model to provide a more complete representation of surface hydrologic dynamics. Here MODHMS© (developed by HydroGeologic Inc, Herndon, VA) was used since it is MODFLOW-based with 3D variably-saturated groundwater flow, 2D overland flow, and 1D channel flow. MODHMS© allows for canopy interception and evapotranspiration so total precipitation and potential evaporation were input to the model for a better estimate of recharge through complete energy and water balance. Singular spectrum analysis (SSA) was used to analyze the temporal response of precipitation, streamflow and groundwater levels from selected points in the model both for MODFLOW and MODHMS© results. This paper demonstrates the use of integrated models for determination of groundwater recharge. Time series analysis proved to be a useful tool in identifying climate response within the watershed.

Braun, Christoph, and Christoph Schoepfer, 2006. **Simulation of Groundwater Driven Flood Risks,** *MODFLOW and More 2006 Managing Groundwater Systems – Conference, Golden, CO., 2006.*

The modelling area is an island in the river Rhine which is protected with dams against overland inundations. During flood events, large parts of the island are under artesian conditions and huge amounts of groundwater can leak to the surface. The purpose of the presented study is to analyse under which hydrological conditions this leakage can lead to flood risks for an industrial plant on the island. Critical hydrological conditions (peak and history) for inundation are derived from simulations of historical and artificial flood events. For this conditions flood propagation in the industrial plant is computed using a fully coupled groundwater - overland flow model. Together with the hydrological study this is used for risk analysis.

Deschaine, L. M., V. Guvanasen, J. D. Pinter, and L. R. Townley (2011). **Optimised Planning for Management of Integrated Surface Water and Groundwater Systems.** *The 34th IAHR World Conference, Brisbane, Australia, 26 June – 1 July, 2011*

Operations managers responsible for mining, water resources, and environmental remediation projects are looking for tools that will help them find solutions to complex planning challenges. As diverse as these industries are, they share a need for an integrated simulation-optimisation approach capable of handling the physics of fully coupled surface and subsurface water flow and chemical transport systems. This paper presents such a toolbox, PBMOTM, which uses physics-based simulators (e.g., MODHMS® and MODFLOW-SURFACT™) to represent chemical and energy transport processes (as well as water flow) and supports integrated analysis of deterministic/stochastic surface water/groundwater flow and transport of multiple contaminants in density-dependent and non-isothermal environments. Optimisation is then performed using HGL-OptTM, a tool that seamlessly communicates with physics-based models during the optimisation calculations. Applications of the proposed approach include dewatering in the mining industry, multiple-source allocation of water resources, and environmental remediation of contaminated sites.

Deschaine, Larry M., Varut Guvanasen, Don DeMarco, Xinyu Wei, János D. Pintér (2010). **Comprehensive Optimal Management Planning of Integrated Aquifer and Surface Water Resource Systems.** *7th Annual International Symposium on Managed Aquifer Recharge Abu Dhabi, 9 - 13 October 2010.*

Regional water resource managers are increasingly looking for tools to provide answers to planning issues related to the inter-relationship of aquifer and surface-water quantity and quality conditions. These issues include the competing aspects of water allocation to activities (agriculture, reservoirs, ecology and the environment), as well as potential future planning scenarios involving resource dependability and quality in the face of climate change. Hence, there is a need for an integrated simulation-optimization approach (and its computer based implementation) that has the capability of handling the physics of the fully-coupled surface and subsurface water flow and chemical transport systems combined with global scope nonlinear optimization. This presentation focuses on such a tool. The physics of water flow, chemical and other material transport is described using the integrated surface water-aquifer simulator MODHMS and the MODFLOW-SURFACT code. These tools implement our comprehensive conjunctive analysis of surface water and aquifers, including recharge, pollutant transport, salt-water intrusion, brine disposal and energy (heat) transport. The optimization is performed using an extension of the Lipchitz Global Optimization (LGO) software that seamlessly communicates with the physics-based models in the optimization calculations. LGO is a derivative-free global (as well as local) optimization tool, here extended towards handling nonlinear models which are computationally expensive to calculate. The presentation discusses MODHMS, MODFLOW-SURFACT and LGO, and the value of optimizing the fully integrated physics based flow system. This is an advancement over other approaches such as those that treat the physics as either individual parts (such as only groundwater resources), or which used simplified (linearization or lumped parameter) representations of the underlying physical processes and/or those approaches which use only local optimization. The simulator and optimization modules have been developed or enhanced through collaboration by researchers at HydroGeoLogic, Chalmers University of Technology, and Özyeğin University.

Deschaine, Larry M., Peter Huyakorn, Varut Guvanasen, and Theodore Lillys (2009). **FTMO: The Advancement of International Efforts in Environmental Simulation, Machine Learning and Optimization Produces an Optimal, Active and Responsive Environmental Response and Remediation Project Planning & Implementation Tool-kit.** *NIDA Environment, Energy, & Sustainability Symposium & Exhibition, 2009.*

The next generation of the Flow, Transport and Management Optimization Tool-kit is presented. This tool kit provides a realistic approach to environmental remediation cost savings leading to optimized contaminated site response and remediation decisions. FTMO components have been peer reviewed – the FTMO approach has been deployed at sites for DOE, DoD and USEPA. The advancement discussed herein is a non-trivial extension of the previous successful applications. The models used now include fully integrated surface and groundwater flow and transport. The management criterion is formally included. Any of the physical or management processes and constraints can be known with or without certainty. Its applicability includes ground and surface water plume tracking, long-term monitoring optimization, optimal remedial design and optimal source finding. The tool kit is designed to be model independent, and can be connected with any flow and transport simulator. This design facilitates the deployment of a unique blend of physics-based simulators with machine learning, expert systems and formal optimization techniques. It now handles more complex problems than heretofore possible using conventional or previous approaches.

Doherty, J., 2001. **Improved Calculations for Dewatered Cells in MODFLOW.** *Ground Water, Vol. 39, No. 6, pp. 863-869.*

Use of the United States Geological Survey ground water flow model MODFLOW is often hampered by the occurrence of "dry cells." While MODFLOW allows such cells to "rewet" in the course of a simulation, stability of the heads solution process is often problematical with rewetting functionality operative. In many cases of practical interest (particularly in mining applications), MODFLOW simply fails to converge. However by making a number of adjustments to the MODFLOW Block-Centered Flow package, it is possible to overcome this problem in many instances of MODFLOW deployment. These adjustments are such as to allow a layer to transmit water, albeit with a vastly reduced transmissivity, even if the water level in that layer is below its base. With these alterations MODFLOW cells can remain active even if they lie within the unsaturated zone.

Testing of the code has demonstrated its ability to perform well in situations where performance of the unmodified MODFLOW is degraded by the necessity to dry and rewet cells. Comparison of heads calculated using the modified MODFLOW with those calculated using MODFLOW-SURFACT™ (a MODFLOW-based code developed by HydroGeoLogic Inc. that prevents the occurrence of dry cells through use of pseudo soil functions) reveals near-identical results between the two codes. Comparison with analytical solutions of water table location also reveals near coincidence. An example of one such application is presented herein.

Fairbanks Jeffrey, Sorab Panday and Peter S. Huyakorn, 2001. **Comparisons of Linked and Fully Coupled Approaches to Simulating Conjunctive Surface/Subsurface Flow and their Interactions.** *Proceedings MODFLOW 2001 Conference, Golden, Colorado, September 11-14. PP. 356-361.*

Surface water flow and subsurface flow have traditionally been investigated separately and simulators have been developed over the years, to model each of these systems. Growing interest in conjunctive water management, and need for simulations of surface/subsurface flow and their interactions has lead to the linking of models of the respective domains. The surface and subsurface domains may be coupled in a time-lagged manner or in an iterative fashion. Further, the coupling may be performed in terms of the interface heads, or in terms of the interaction fluxes. Finally, several sub-time steps of simulation may be performed for the surface water domain before proceeding to one large time-step for the subsurface domain due to the temporal scale differences for flow within the two regimes.

A comparison of numerical accuracy, efficiency and robustness of the various linked approaches is performed here, along with the fully coupled approach. It is determined that the fully coupled approach is robust, and efficient for all simulation cases, followed by head coupling with iterations. Care should be taken in selecting a small-enough time step size for non-iterative decoupled approaches, since no criterion exists to determine the adequacy of the time-step size and erroneous results may be produced with large time-step sizes. The decoupled approaches perform comparably with the fully coupled approach only when interaction fluxes between the surface and subsurface are small.

Gabora Michael, Vivek Bedekar, Bill Linderfelt and Andy Davis, 2006. **Integration of the LAK3 Package into MODFLOW-SURFACT™ to Simulate an Ephemeral Pit Lake, Northern California,** *MODFLOW and More 2006 Managing Groundwater Systems – Conference, Golden, CO., 2006. V.2, p.705.*

The LAK3 package was integrated into MODFLOW-SURFACT™ in order to solve an ephemeral pit lake problem associated with a proposed hard rock quarry in northern California. Utilization of MODFLOW-SURFACT™ permitted free movement of the steeply dipping water table in unconfined layers adjacent to the dewatered quarry. The LAK3 package was required because it allows for efficient drying and rewetting of lake cells. As a result of the climate and low permeability of the bedrock in the vicinity of the quarry, an ephemeral pit lake was expected to form upon cessation of mining activities. The rewetting procedure in the LAK3 package uses the average hydraulic head in the cells underlying the lake cells, which, due to steep hydraulic gradients associated with the pit, created unrealistic starting heads during rewetting. A modified rewetting procedure was implemented in the LAK3 package to accurately simulate shallow ephemeral ponding in the reclaimed quarry whereby the lake stage was set to the quarry bottom plus a nominal head of 0.05 feet.

Gallagher, M. and Doherty, J. 2006. **Parameter interdependence and uncertainty induced by lumping in a hydrologic model.** *Water Resources Research, doi:10.1029/2006WR005347*

Throughout the world, watershed modeling is undertaken using lumped parameter hydrologic models that represent real-world processes in a manner that is at once abstract, but nevertheless relies on algorithms that reflect real-world processes and parameters that reflect real-world hydraulic properties. In most cases, values are assigned to the parameters of such models through calibration against flows at watershed outlets. One criterion by which the utility of the model and the success of the calibration process are judged is that realistic values are assigned to parameters through this process. This study employs regularization theory to examine the relationship between lumped parameters and corresponding real-world hydraulic properties. It demonstrates that any kind of parameter lumping or averaging can induce a substantial amount of "structural noise," which devices such as Box-Cox transformation of flows and autoregressive moving average (ARMA) modeling of residuals are unlikely to render homoscedastic and uncorrelated. Furthermore, values estimated for lumped parameters are unlikely to represent average values of the hydraulic properties after which they are named and are often contaminated to a greater or lesser degree by the values of hydraulic properties which they do not purport to represent at all. As a result, the question of how rigidly they should be bounded during the parameter estimation process is still an open one.

Guha, H. and Panday, S., 2005, **Application of a Density-Dependent Numerical Model to Assess Salinity Intrusion in the Biscayne Bay Aquifer, Northern Miami-Dade County, Florida.** *EOS, Transactions, Joint Assembly, American Geophysical Union, New Orleans, Louisiana. May 23-27, 2005.*

Miami-Dade County is located at the Southeastern part of the State of Florida adjoining the Atlantic coast. The sole drinking water source is the Biscayne Aquifer, which is an unconfined freshwater aquifer, composed of marine limestone with intermediate sand lenses. The aquifer is highly conductive with hydraulic conductivity values ranging from 1,000 ft/day to over 100,000 ft/day in some areas. Saltwater intrusion from the coast is an immediate threat to the freshwater resources of the County. Therefore, a multilayer density-dependent transient groundwater model was developed to evaluate the saltwater intrusion characteristics of the system. The model was developed using MODHMS©, a finite difference, fully coupled groundwater and surface water flow and transport model. The buoyancy term is included in the equation for unconfined flow and the flow and transport equations are coupled using an iterative scheme. The transport equation was solved using an adaptive implicit total variation diminishing (TVD) scheme and anisotropy of dispersivity was included for longitudinal, transverse, vertical transverse, and vertical longitudinal directions. The model eastern boundaries extended approximately 3.5 miles into the Atlantic Ocean while the western boundary extended approximately 27 miles inland from the coast. The northern and southern boundaries extend 6 miles into Broward County and up to the C-100 canal in Miami-Dade County respectively. Close to 2 million active nodes were simulated, with horizontal discretization of 500 feet. A total of nine different statistical analyses were conducted with observed and simulated hydraulic heads. The analysis indicates that the model simulated hydraulic heads matched closely with the observed heads across the model domain. In general, the model reasonably simulated the inland extent of saltwater intrusion within the aquifer, and matched relatively well with limited observed chloride data from monitoring wells along the coast. Saltwater intrusion in the Biscayne aquifer is the result of a combination of natural variations in recharge, evapotranspiration, ground-water withdrawals from the aquifer, and relative canal stages in comparison to tidal stages in the Biscayne Bay. Pre- and post wellfield pumpage scenarios were conducted to determine the effect of wellfield pumpage on saltwater intrusion. The model is being used for future water supply management scenarios and for evaluating the best placement of saltwater intrusion monitoring wells along the coast.

Guvanasen, Varut, Xinyu Wei, Deyang Huang, Dilip Shinde, and Rene Price (2011). **Application of MODHMS to Simulate Integrated Water Flow and Phosphorous Transport in a Highly Interactive Surface Water Groundwater System along the Eastern Boundary of the Everglades National Park, Florida.** *MODFLOW and More 2011: Integrated Hydrologic Modeling The Colorado School of Mines, Golden, Colorado. June 5-8, 2011*

MODHMS is a state-of-the-art MODFLOW-based Hydrologic Modeling System that performs comprehensive simulations of integrated surface-water/groundwater flow and multiple contaminants in density-dependent and non-isothermal environments. A three-dimensional integrated surface water groundwater flow and dual-porosity transport model, based on MODHMS was developed and used to investigate the groundwater flow pattern and water quality as part of the MODWATER C-111 Project in response to the operations of the system of canals, levees, and pumping stations, as well as climatic conditions.

The MODWATER C-111 project is intended to provide both flood control and ecological restoration functions to Everglades National Park (ENP) by creating and maintaining a hydrologic barrier (detention areas) along the eastern boundary of the Park to control outgoing seepage water. Major ENP concerns in this area are the distribution and transport of water-borne phosphorus (P) which is pumped into the detention areas from a major influent canal. Available physico-chemical data and historical records of potentiometric elevation, canal flow rate, and total P from 2000 to 2007 were used to develop and calibrate the integrated flow and transport model for the detention areas. The model simulations were used to examine the movement of pumped water and associated total P in the detention areas and their surroundings. In this paper, model development and calibration will be described. Results from sensitivity analyses and simulations will be discussed.

Guvanasen, Varut, Xinyu Wei, Deyang Huang, Dilip Shinde, and Rene Price (2011). **Simulation of Water Flow and Phosphorous Transport in a Highly Interactive Surface Water Groundwater System in the S332 Detention Areas Upstream of Taylor Slough, Everglades National Park.** *GEER 2010 Greater Everglades Ecosystem Restoration. Naples, FL. July 12-16, 2010*

The MODWATER C-111 project is intended to provide both flood control and ecological restoration functions to ENP. The project seeks to minimize drainage of ENP marshes by creating and maintaining a hydrologic barrier along the eastern boundary of the Park. Water is pumped from the L-31N canal west into the S332 detention areas to create a hydrologic barrier to maintain water levels in ENP and to reduce the west-to-east hydraulic gradient, which drains the Rocky Glades region of ENP. On the southeastern neighboring areas of ENP in C-111 canal basin, a number of hydraulic structures exist that regulate the surface and groundwater flow patterns. Surface water is highly interactive with groundwater and the area is underlain by the highly transmissive Biscayne Aquifer. Major ENP concerns in this area are the distribution and transport of phosphorus (P). The main sources of P into ENP are the L-31N and C-111 canals from where water-borne P is pumped into the S 332BN, S-332BW, S-332C, and S-332D detention areas.

A three-dimensional integrated surface water groundwater flow and transport model, based on MODHMS (HGL 2001), was used to investigate the groundwater flow pattern and water quality in and around detention areas in response to the operations of the system of canals, levees, and pumping stations, as well as climatic conditions. MODHMS is a state-of-the-art MODFLOW-based Hydrologic Modeling System that performs comprehensive simulations of conjunctive surface-water/groundwater flow and chemical transport. MODHMS performs integrated hydrologic analysis using a fully coupled solution of the diffusion wave equations governing overland flow and channel flow with the Richards equation governing unsaturated/saturated groundwater flow. Available data on total P concentration, potentiometric elevation, canal and detention areas stages, and flow through canals between 2000 and 2007 were used as quantitative calibration targets. The model simulations were used to examine of movement of pumped water and associated total P from the detention areas and in the surroundings.

Most of the water and P tend to leave all detention areas in the easterly direction toward the C-111 canal. In the L-31W canal, most of the water (~ 95 %) and P fluxes that enter the Biscayne aquifer migrate in the easterly direction, and the remaining 5 % in the westerly direction, on average. However, the westerly water flow and P migration is episodic, and all the water and water-borne P that flow into the ENP get flushed out to the east eventually. A sensitivity analysis was performed and the results indicate that the two most sensitive transport parameters are distribution coefficient and dual-porosity mass transfer rate. The current model is capable of simulating salient characteristics and long-term trend of P. However, the current model's predictive capability is limited to simulating the behavior of P transport in a macro-scale sense. The major sources of uncertainty in P transport were thought to include: behavior and transport of P in soil and limestone and P Source identification.

Guvanasen, Varut, Vivek Bedekar, Dilip Shinde, and Rene Price (2010). **Development of a Flow and Transport Model in a highly Interactive Surface Water Groundwater System Near Everglades National Park in South Florida, USA.** *7th Annual International Symposium on Managed Aquifer Recharge Abu Dhabi, 9 - 13 October 2010.*

Everglades National Park (ENP) in south Florida, with the largest subtropical wilderness in the United States, was created to protect a fragile ecosystem instead of safeguarding a geographic feature. In 2000, the U.S. Congress authorized the Comprehensive Everglades Restoration Plan (CERP), the largest environmental restoration effort in history, to enhance the Everglades wetlands and associated lakes, rivers, and bays in south Florida. Along the southeastern adjoining areas of ENP in C111 canal basin, a number of hydraulic structures have been constructed to help regulate the groundwater flow pattern within ENP. In this area, surface water is highly interactive with groundwater. This area is underlain by Biscayne Aquifer, a highly transmissive aquifer. Phosphorus distribution and transport are also of concern in this area. A three-dimensional integrated surface water groundwater flow and transport model was developed and used as an analytical and management tool to investigate the operations and the impacts due to the construction of levees, canals, pumping stations, and detention basins on the groundwater flow pattern and water quality. The developed model simulates transient surface water groundwater flow and transport in double-porosity porous media for the southeastern boundary area of ENP in response to the operations of the system of canals, levees, and pumping stations, as well as climatic conditions. This model covers an area of more than 400 square kilometers and was calibrated to a set of pre-specified calibration criteria. Available data of total phosphorus concentration, potentiometric elevation, canal and detention basin stages, and flow through canals between 2000 and 2007 were used as quantitative calibration targets. Details of model development and calibration and sensitivity analysis results are presented and discussed.

Guvanasen, Varut, Markus Himml, and Bettina Buechler (2009). **Simulation of Kinetic-Limited Degradation of Multi-Component Hydrocarbons with particular consideration on the supply of electron acceptors.** *International Symposium on Efficient Groundwater Resources Management "The Challenge of Quantity and Quality for Sustainable Future", February 16-21, 2009. Bangkok, Thailand*

Modeling natural attenuation processes of hydrocarbons in groundwater systems is normally performed with numerical methods. Clement et al. (1997) developed a spatially variable reactive transport code (RT3D) which, among others, allows for a kinetic-limited degradation of a single or averaged property hydrocarbon using multiple electron acceptors in sequential order. In some cases, e.g., when fresh water from surface-water bodies is entering the system or flow directions are significantly changing, this approach might not be sufficient, because of possible mixing processes with alternating redox conditions within the plume. An enhancement of the RT3D code was developed for the groundwater simulation software MODFLOW-SURFACT Version 3.0. This enhancement enables the inclusion of concomitant inorganic reactions, e.g., the formation of hydrogen sulfide during sulfate reduction and possible subsequent precipitation of iron sulfide which may be oxidized again by other electron acceptors.

MODFLOW-SURFACT 3.0 was applied to a site in which a 60-year-old hydrocarbon spill is being investigated to evaluate options for remedial actions. The volume of the spill is greater than 3,000 cubic meters of non-aqueous phase liquid (NAPL). The NAPL consists of multiple hydrocarbon species with different properties and kinetic-limited decay characteristics. The site is characterized by a complex three-dimensional hydrogeologic setting between two port basins with significant water table fluctuations, which induce highly spatio-temporally variable horizontal and vertical flow gradients and extensive hydrodynamic dispersion in the contaminated area. Surface water is oxygen-rich, but does not reach the center of the contamination plume which is mainly characterized by iron reduction, sulfate reduction and methanogenesis. Only in the region of the seam of the contamination can oxygen and nitrate contribute to hydrocarbon decay significantly. On the transport path towards the center of the plume oxygen and nitrate are reduced by ferrous iron and significant amounts of iron sulfide which have been produced during the last decades. Objectives of the modeling, which is based on field data, are: (i) to estimate the mass transfer rate of hydrocarbons into the surface water, and (ii) to quantify approximately natural degradation processes; so that appropriate actions may be planned.

The enhanced reaction model and site model development will be presented. Preliminary results from the simulations will also be presented and discussed.

Guvanasen, Varut, Ming-Shu Tsou, Xinyu Wwi, and Patrick Burger (2009). **Development Of a Large-Scale Three-Dimensional Density-Dependent Saltwater Intrusion Model for the Tiger Bay Area, Florida, USA.** *International Symposium on Efficient Groundwater Resources Management "The Challenge of Quantity and Quality for Sustainable Future", February 16-21, 2009. Bangkok, Thailand.*

In the East-Central Florida region, public supply demands are expected to double between 1995 and 2025. The Tiger Bay area, which is situated along the coastline of the East-Central Florida region of the St Johns River Water Management District, has been identified as a Priority Water Resource Caution Area, because of its predicted inability to meet 2025 water-supply demands from traditional groundwater supply sources without unacceptable impacts on water quality, wetlands, and other natural resources. For the purposes of water supply assessment, two factors were evaluated by the District: water quality trends and increases in groundwater withdrawals. As part of the ongoing evaluation of how increased groundwater withdrawals impact water quality, a density-dependent groundwater flow and transport model was identified as an essential analytical and management tool. Specifically, the model will be used to simulate regional groundwater flow and water quality changes (chlorides) in the aquifer system in response to groundwater withdrawals. To satisfy this requirement, a three-dimensional computer model that simulates variable-density, transient groundwater flow in porous media for the Tiger Bay area was developed. This model covers an area of more than 2 000 square kilometers. The calibration of the model was conducted in two stages: predevelopment calibration (circa 1936), and transient calibration (1936 to 1999). The model was calibrated to a set of pre-specified calibration criteria. Available chloride, and potentiometric data were used as quantitative calibration targets. Additional data, such as altitudes of isochlors and published potentiometric distribution for pre-development, were also used for confirmatory purposes. The calibrated model was then utilized to perform a predictive simulation to evaluate the effects of projected pumping rates through the year 2025. Results from predictive simulation runs indicate the migration of saltwater interface toe is expected to on the order of one kilometer.

This paper presents the details of model development and calibration. Results of predictive simulations and sensitivity analysis are also discussed.

Hopmans, J. W., G. Schoups, K. K. Tanji, and W. W. Wallender (2005). **Integrated modeling of regional-scale flow and reactive salt transport in the western San Joaquin Valley.** *Eos Trans. AGU, 86(18), Jt. Assem. Suppl., Abstract H21B-07.*

An integrated model of regional-scale subsurface flow and reactive salt transport and its application to the western San Joaquin Valley study area is presented. The integrated model uses the MODHMS© model to simulate three-dimensional subsurface flow and transport, and couples it to the major ion chemistry modules of the UNSATCHEM model. Unique features of the integrated model include the full coupling of the vadose zone and groundwater systems, and the accounting for major ion chemistry effects on soil and groundwater salinization. The model was applied to the western San Joaquin Valley study area to simulate changes in regional-scale soil and groundwater salinization that occurred over the last 50 years. Model simulation results were compared to historical observations of water table depths, groundwater pumping, subsurface drainage, and soil and groundwater salinity. Based on the general correspondence between observed and simulated relationships it was concluded that these processes are adequately represented in the model.

Hopmans, J. W., and G. Schoups (2005). **Regional-scale hydrologic modeling of flow and reactive salt transport in the San Joaquin Valley.** *Eos Trans. AGU, 86(52), Fall Meet. Suppl., Abstract H41G-01, INVITED.*

A hydro-salinity model was developed to integrate subsurface hydrology with reactive salt transport for a 1,400 km2 study area in the San Joaquin Valley, CA. For the first time, such a modeling framework was used to reconstruct historical changes in salt storage by irrigated agriculture over the past 60 years. We show that patterns in soil and groundwater salinity were caused by spatial variations in soil hydrology, the switching from local groundwater to snowmelt water as the main irrigation water supply, and by occasional droughts. Gypsum dissolution was a critical component of the regional salt balance. Although results show that the total salt input and output were about equal for the past 20 years, the model also predicts salinization of the deeper aquifers, thereby questioning the sustainability of irrigated agriculture.

Hopmans, J. W., and G. Schoups 2006. **Integrated Modeling of Regional-Scale Flow and Reactive Salt Transport in the Western San Joaquin Valley.** *MODFLOW and More 2006 Managing Groundwater Systems – Conference, Golden, CO., 2006. V.2, p.609.*

The sustainability of irrigated agriculture in many arid and semi-arid areas of the world is at risk because of a combination of several interrelated factors, including lack of fresh water, lack of drainage, the presence of high water tables, and salinization of soil and groundwater resources. Nowhere in the United States are these issues more apparent than in the San Joaquin Valley of California. A solid understanding of salinization processes at regional spatial and decadal time scales is required to evaluate the sustainability of irrigated agriculture. A hydro-salinity model was developed to integrate subsurface hydrology with reactive salt transport for a 1,400 km2 study area in the San Joaquin Valley of California. The model was used to reconstruct historical changes in salt storage by irrigated agriculture over the past 60 years. We show that patterns in soil and groundwater salinity were caused by spatial variations in soil hydrology, the change from local groundwater to snowmelt water as the main irrigation water supply, and by occasional droughts. Gypsum dissolution was a critical component of the regional salt balance. Although results show that the total salt input and output were about equal for the past 20 years, the model also predicts salinization of the deeper aquifers, thereby questioning the sustainability of irrigated agriculture.

Huang, Deyang, Xinyu Wei, Prashanth Khambhammettu, Jan Kool, and Ming-shu Tsou (2011). **A Methodology to Simulate Streamflow Losses and Groundwater – Surface Water Interactions due to Karst Sink Holes.** *MODFLOW and More 2011: Integrated Hydrologic Modeling The Colorado School of Mines, Golden, Colorado. June 5-8, 2011*

The Peace River is the major river system in central Florida. Portions of the Upper Peace River are characterized by numerous karst features in or near the river channel. These karst features provide a direct hydraulic connection between the Peace River and the underlying Intermediate and Upper Floridan aquifers. Historically, streamflow in the Upper Peace River received significant contributions from spring flow. However, since the middle of the 20th century, flowing wells and springs have diminished and ceased flowing as groundwater levels have declined. Associated with this decline, karst features now act as sinks for flow in the Peace River during dry periods.

As part of a project to develop a fully integrated groundwater-surface water model of the entire Peace River basin, karst flow losses were simulated using the node-link feature of MODHMS. MODHMS is a MODFLOW-based Integrated Surface water/groundwater Modeling System. Direct hydraulic links between CHF channel segments representing the Peace River and the underlying grid blocks representing the subsurface were incorporated in the model to simulate the presence of karst conduits. The methodology accounts for the head dependence of stream flow losses as well as the storage of subsurface karst cavities which can be important in the transient response of the rate of flow loss to changes in stream flow rate and groundwater heads.

Detailed comparisons between simulated karst flow losses from Peace River modeling between simulated results and USGS observations were conducted. The comparison showed that under hydrologically similar stream flow conditions, the PRIM model can reproduce observed karst losses of stream quite well. The comparisons also showed that karst features as simulated in the model reproduced the characteristic of stream flow losses under low-flow conditions.

Hyun Yunjung, Kang-Kun Lee, and Yoon Young Kim, 2006. **Consequence of Groundwater-Surface Water Interactions for Groundwater Contamination in a Variably Saturated Aquifer,** *MODFLOW and More 2006 Managing Groundwater Systems – Conference, Golden, CO., 2006.*

The interactions between groundwater and contaminated surface water may influence on groundwater contamination. In urban environments, the aquifer located around a stream often becomes variably saturated due to variation of recharge rates, transpiration, domestic pumping and seepage into some underground facilities. The variation of aquifer saturation may change the degree of groundwater-surface water interactions. Through stream depletion, contaminants dissolved in a stream migrate into adjacent groundwater systems, mix with groundwater, and deteriorates groundwater quality. The extent of associated groundwater contamination is determined by coupled flow and transport modeling. For this study, numerical modeling is performed with a computer code for coupled flow and transport simulations in variably saturated aquifers, MODFLOW-SURFACT™ (HydroGeoLogic, Inc., 1996). Simulation results allow the spatial delineation of areas where groundwater-surface water interaction occurs. The extent of simulated groundwater contamination was shown to be more significant under moderately and highly saturated conditions than slightly saturated conditions. Simulations revealed that groundwater contamination under slightly saturated conditions is as significant as moderately or highly saturated conditions in a long term development of stream depletion. This study presents a preliminary base for management and assessment of water resources in the variably saturated groundwater system adjacent to an urban stream.

Johnson, R. L., R. B. Thoms, and J. S. Zogorski, 2003. **Effects of Daily Precipitation and Evapotranspiration Patterns on Flow and VOC Transport to Groundwater along a Watershed Flow Path.** *Environmental Science & Technology, Vol. 37, No. 21, pp. 4944-4954*

MTBE and other volatile organic compounds (VOCs) are widely observed in shallow groundwater in the United States, especially in urban areas. Previous studies suggest that the atmosphere and/or nonpoint surficial sources could be responsible for some of those VOCs, especially in areas where there is net recharge to groundwater. However, in semi-arid locations where annual potential evapotranspiration can exceed annual precipitation, VOC detections in groundwater can be frequent. VOC transport to groundwater under net discharge conditions has not previously been examined. A numerical model is used here to demonstrate that daily precipitation and evapotranspiration (ET) patterns can have a significant effect on recharge to groundwater, water table elevations, and VOC transport. Ten-year precipitation/ET scenarios from six sites in the United States are examined using both actual daily observed values and "average" pulsed precipitation. MTBE and tetrachloroethylene transport, including gas-phase diffusion, are considered. The effects of the precipitation/ET scenarios on net recharge and groundwater flow are significant and complicated, especially under low-precipitation conditions when pulsed precipitation can significantly underestimate transport to groundwater. In addition to precipitation and evapotranspiration effects, location of VOC entry into the subsurface within the watershed is important for transport in groundwater. This is caused by groundwater hydraulics at the watershed scale as well as variations in ET within the watershed. The model results indicate that it is important to consider both daily precipitation/ET patterns and location within the watershed in order to interpret VOC occurrence in groundwater, especially in low-precipitation settings.

Kalf, Frans and Donald R Woolley, 2005. **Applicability and Methodology of Determining Sustainable Yield in Groundwater Systems,** *Theme issue Journal of Hydrogeology Vol 13, Number 1 - March 2005 pages 295-312*

There is currently a need for a review of the definition and methodology of determining sustainable yield. The reasons are: (1) current definitions and concepts are ambiguous and non-physically based so cannot be used for quantitative application, (2) there is a need to eliminate varying interpretations and misinterpretations and provide a sound basis for application, (3) the notion that all groundwater systems either are or can be made to be sustainable is invalid, (4) often there are an excessive number of factors bound up in the definition that are not easily quantifiable, (5) there is often confusion between production facility optimal yield and basin sustainable yield, (6) in many semi-arid and arid environments groundwater systems cannot be sensibly developed using a sustained yield policy particularly where ecological constraints are applied. Derivation of sustainable yield using conservation of mass principles leads to expressions for basin sustainable, partial (non-sustainable) mining and total (non-sustainable) mining yields that can be readily determined using numerical modelling methods and selected on the basis of applied constraints. For some cases there has to be recognition that the groundwater resource is not renewable and its use cannot therefore be sustainable. In these cases, its destiny should be the best equitable use.

Khambhammettu, Prashanth, Jan Kool, Ming-Shu Tsou, Peter Huyakorn, and Michael Beach (2009). **Modeling the Surface-Water Groundwater Interactions in the Peace River Basin, Florida, USA.** *International Symposium on Efficient Groundwater Resources Management "The Challenge of Quantity and Quality for Sustainable Future", February 16-21, 2009. Bangkok, Thailand.*

The Peace River begins in central Florida at the confluence of the Peace Creek Drainage Canal and Saddle Creek and flows south 105 miles to the Charlotte Harbor Estuary. The Peace River drainage basin is approximately 2350 square miles in area. A long term decline in stream flows and groundwater potentiometric levels has been observed in the region and the causes are complex. Land-use changes altering runoff, surface-water storage, recharge and evapotranspiration patterns, increased groundwater and surface-water withdrawals and climatic changes are some of the causes for this decline. The South West Florida Water Management District (SWFWMD) has funded the development of the Peace River Integrated Model (PRIM) to assess the effects of land use, water use, and climatic changes on stream flows and to evaluate the effectiveness of various management alternatives for restoring stream flows. The first phase of model development involves the Saddle Creek sub-basin, located in the northern part of the watershed. The main objective of the Saddle Creek Basin Integrated Model (SCBIM) is to create an integrated surface water / groundwater (SW/GW) model of the Saddle Creek sub-basin, and to evaluate model performance.

The model was developed using MODHMS and is being calibrated and verified against various stream flow, lake stage and groundwater level data over a period of 9 years from February 1994 to December 2002. The surficial domain of the model was parameterized for the various land use categories rather than on a grid-block basis. These calibrated parameter values (specifically, the leakance, Manning's friction and crop coefficient of different land use types) can be directly extended to the PRIM study. Furthermore, the calibration and sensitivity experience can also be extended to the PRIM study.

Lessons learned from development and calibration of the SCBIM will be valuable in development and calibration of the basin-wide PRIM model. Further, calibrated parameters for various soil types and land use categories will be extended to the entire PRIM domain.

Lee, Sam, and Sorab Panday, 2006. **Three-Dimensional Seepage Analysis through Fordyce Dam.** *Joint Eighth Federal Interagency Sedimentation Conference and Third Federal Interagency Hydrologic Modeling Conference April 2 – 6, 2006 Silver Legacy Hotel, Reno, Nevada*

A three-dimensional model was developed for analyzing the seepage through Fordyce Dam. A two-dimensional analysis of seepage through the dam under-predicts seepage fluxes by a factor of 5 when established hydraulic conductivity values are used for the rock materials. The three-dimensional model provides similar seepage fluxes to the two-dimensional model, when identical conditions are compared. The three-dimensional model was used to explore various alternatives that could be the cause of the observed seepage fluxes, followed by analyses that can guide field monitoring activities to reduce the uncertainty between these alternatives.

Leppert, Shawn, 2006. **Hydraulic Property Distribution Estimation through Groundwater Modeling of the Observed Effects from "Uncontrolled" Resident Hydraulic Stress,** *MODFLOW and More 2006 Managing Groundwater Systems – Conference, Golden, CO., 2006. V.2, p. 496.*

In the vast majority of numerical groundwater flow analyses that I review, conventional calibration techniques are applied. The models are calibrated to a flow field which is assumed to be in equilibrium and compare to field data collected from a "controlled" 24, 48, or 72 hour hydraulic stress test. During the last few years, I have had success using data that represent transient, "uncontrolled" hydraulic stresses to aid in the calibration of complex groundwater flow models. For the purposes of this paper, I include both natural and anthropogenic resident hydrologic features as types of transient "uncontrolled" hydraulic stresses. I share my experiences calibrating complex groundwater flow models using three such hydraulic stresses. The first experience outlines how hydraulic stress response data, inadvertently collected for a river's flood stage, was used to estimate the porous media properties of shallow waterbearing hydrogeologic units hydraulically connected to the river. Flood waters induced a large magnitude stress which was detected in every monitoring well on-site. This stress revealed significantly more information about the shallow subsurface than the "controlled" hydraulic stress test. In the second example, a hydraulic stress produced by a tidally influenced river located along the site property boundary is described. Similar to the first example, the transient stress produced by the tides was used to delineate the hydraulic connectivity between the shallow water-bearing units and the river, a major influence on the groundwater flow regime at the site. The final experience I share in this paper is one I had evaluating a designed, "controlled" hydraulic stress test where monitoring was performed for a relatively long period before and after the stress test was applied. During the periods before and after the stress test, groundwater monitoring data captured precipitation events and variations in the site's water supply extraction that were used to assist in the calibration of the site's groundwater flow model. Resident, transient, hydrologic features do exert significant stress on local groundwater flow regimes. Examination of a water-bearing unit's response to these "uncontrolled" stresses can provide great insight into the 3- dimensional distribution of porous media properties. These type stresses are often present in the shallow subsurface; one only needs to monitor their effects to benefit from the information available.

Panday, Sorab, and Peter. S. Huyakorn, 2004. **A Fully-Coupled Physically-Based Spatially Distributed Model for Evaluating Surface/Subsurface Flow.** *Advances in Water Resource Vol. 27, pp. 361 - 382.*

A physically-based, spatially-distributed model is presented for simulation of surface/subsurface flow and the interactions between these domains. The model is designed for practical application to a wide variety of hydrologic evaluations, at various scales of simulation. The system is represented by the three-dimensional saturated–unsaturated flow equation for the subsurface, coupled with the diffusion wave equation for areal overland flow, both of which are coupled with the diffusion wave equation for flow through a network of streams and channels, including hydraulic structures. Ground surface unevenness at the grid scale is incorporated via the concept of detention storage, and thick vegetation or urban features are included via an obstruction storage exclusion term. Evapotranspiration from the surface and subsurface are modeled using land cover and climatic factors to define the complete water budget using a physically-based formulation. The system of equations is discretized using a fully implicit procedure, with the Newton–Raphson method to handle non-linearities efficiently. Robustness, stability and accuracy of solution are obtained for a wide variety of cases including dry systems and large surface/subsurface interaction fluxes. Adaptive time-stepping schemes and under-relaxation formulas further alleviate the computational burden. Verification and application examples demonstrate the need for a rigorous, fully-coupled solution to the set of equations, for complete hydrologic-cycle analysis.

Panday, Sorab, and Brian McGurk, 2006. **An Integrated Surface Subsurface Model in Western Orange and Seminole Counties, Florida,** *Joint Eighth Federal Interagency Sedimentation Conference and Third Federal Interagency Hydrologic Modeling Conference April 2 – 6, 2006Silver Legacy Hotel, Reno, Nevada*

Population growth of Florida in recent years has resulted in a significant increase in the demand for water, with potential impacts of continually increasing withdrawals from the Floridan Aquifer System (FAS) occurring on the surface-water regime and the water-table aquifer. Previous modeling studies have focused on the FAS impacts but raise important issues regarding the surficial domain. The current study addresses the conjunctive issue of impacts of water withdrawals from any regime on the surface and subsurface regimes of the hydro-cycle, in Western Orange and Seminole Counties (WOSC). An integrated surface-water groundwater model has been developed for the analysis by telescopic refinement of the existing regional groundwater flow model for East Central Florida. The Surficial Aquifer System is conceptualized in greater detail to capture the relevant physics that may dominate at the smaller scale of investigation. The unsaturated and surficial flow domains have been rigorously treated, to extend the groundwater flow analysis into a conjunctive framework. The soils map of the region was used to parameterize the unsaturated flow properties and soil-dependent evapotranspiration parameters such as field capacity and wilting point. The land-use, land cover map delineated surficial flow properties such as infiltration characteristics and surficial flow roughness, as well as plant-dependent evaporation / evapotranspiration parameters like Leaf Area Index. The extensive surface drainage features that exist within the domain were also integrated into the model from available databases developed by the counties for flood management. Model development, parameterization, calibration, and significant results are discussed in the context of making improved long-term water management decisions using a conjunctive modeling approach in terms of meeting the increased supply goals as well as sustaining other surface water interests.

Peng, W-S., D. R. Hampton, L. F. Konikow, K. Kambham, and J. J. Benegar, 2000. **Can Contaminant Transport Models Predict Breakthrough?** *Groundwater Monitoring and Remediation, Vol. 20, No. 4, pp. 104-113.*

A solute breakthrough curve measured during a two-well tracer test was successfully predicted in 1986 using specialized contaminant transport models. Water was injected into a confined, unconsolidated sand aquifer and pumped out 125 feet (38.3 m) away at the same steady rate. The injected water was spiked with bromide for over three days; the outflow concentration was monitored for a month. Based on previous tests, the horizontal hydraulic conductivity of the thick aquifer varied by a factor of seven among 12 layers. Assuming stratified flow with small dispersivities, two research groups accurately predicted breakthrough with three-dimensional (12-layer) models using curvilinear elements following the arc-shaped flowlines in this test.

Can contaminant transport models commonly used in industry, that use rectangular blocks, also reproduce this breakthrough curve? The two-well test was simulated with four MODFLOW-based models, MT3D (FD and HMOC options), MODFLOWT, MOC3D, and MODFLOW-SURFACT.

Using the same 12 layers and small dispersivity used in the successful 1986 simulations, these models fit almost as accurately as the models using curvilinear blocks. Subtle variations in the curves illustrate differences among the codes. Sensitivities of the results to number and size of grid blocks, number of layers, boundary conditions, and values of dispersivity and porosity are briefly presented. The fit between calculated and measured breakthrough curves degenerated as the number of layers and/or grid blocks decreased, reflecting a loss of model predictive power as the level of characterization lessened. Therefore, the breakthrough curve for most field sites can be predicted only qualitatively due to limited characterization of the hydrogeology and contaminant source strength.

Schoups, G., J. W. Hopmans, C. A. Young, J. A. Vrugt, and W. W. Wallender (2005). **Multi-criteria optimization of a regional spatially-distributed subsurface water flow model.** *Journal of Hydrology, 311(1-4), 20-48.*

This paper presents the multi-criteria calibration of a regional distributed subsurface water flow model for a 1400 km2 irrigated agricultural area in the western San Joaquin Valley of California. Two global optimization algorithms were used to identify model parameters using data on spatially distributed local water table depth measurements, district-average groundwater pumping and district-average subsurface drainage data. Model parameters that were subjected to calibration included irrigation efficiency, effective drain depth and conductance, crop evapotranspiration correction coefficient, saturated hydraulic conductivity and specific yield values of coarse and fine fractions, and saturated hydraulic conductivity values defining water fluxes across domain boundaries. Using the single-objective function approach, the three measurement types were weighted into a single-objective function for global optimization purposes. Additionally, a three-objective multi-criteria optimization problem was formulated in which no prior weighting of the individual objectives was specified. The single-objective optimization approach resulted in identifiable parameters with relatively small uncertainties, however, most likely values for various optimized parameter approached the outer bounds of their physical-realistic ranges. The normalized weighting of the single-objective function approach emphasized the pumping and drainage data more than the water table depth data. In the multi-objective approach, the objective function of each measurement type was treated independently, so that no subjective preferences were assigned a priori. Within a single optimization run, a Pareto set of solutions was generated, which included the optimal results for each end-member of each of the three objective functions. The results showed a moderate trade-off between pumping and water table predictions, and a slight independence of drainage predictions from the other two measurements. The estimated Pareto set exhibited large parameter uncertainty, indicating possible model structural inadequacies. We further show that the magnitude of prediction uncertainties associated with the Pareto parameter uncertainty is large for making water table predictions, but much smaller for drainage and pumping predictions. Trade-offs between fitting shallow and deep water tables were revealed by considering additional performance criteria for model evaluation, namely BIAS and RMSE values for six water table depth groups. These results point to possible model improvements by spatially distributing some of the model parameters.

Schoups, G., J. W. Hopmans, C. A. Young, J. A. Vrugt, W. W. Wallender, K. K. Tanji, and S. Panday (2005). **Sustainability of irrigated agriculture in the San Joaquin Valley, California.** *Proceedings of the National Academy of Sciences, 102, 15352-15356.*

The sustainability of irrigated agriculture in many arid and semiarid areas of the world is at risk because of a combination of several interrelated factors, including lack of fresh water, lack of drainage, the presence of high water tables, and salinization of soil and groundwater resources. Nowhere in the United States are these issues more apparent than in the San Joaquin Valley of California. A solid understanding of salinization processes at regional spatial and decadal time scales is required to evaluate the sustainability of irrigated agriculture. A hydro-salinity model was developed to integrate subsurface hydrology with reactive salt transport for a 1,400-km2 study area in the San Joaquin Valley. The model was used to reconstruct historical changes in salt storage by irrigated agriculture over the past 60 years. We show that patterns in soil and groundwater salinity were caused by spatial variations in soil hydrology, the change from local groundwater to snowmelt water as the main irrigation water supply, and by occasional droughts. Gypsum dissolution was a critical component of the regional salt balance. Although results show that the total salt input and output were about equal for the past 20 years, the model also predicts salinization of the deeper aquifers, thereby questioning the sustainability of irrigated agriculture.

Schoups, G., J. W. Hopmans, C. A. Young, J. A. Vrugt, and W. W. Wallender (2004). **Parameter uncertainty analysis of a regional subsurface water flow model using single and multi-objective calibration.** *Eos Trans. AGU, 85(47), Fall Meet. Suppl., Abstract H13A-0399.*

Regional-scale modeling of variably-saturated subsurface water flow is affected by uncertainties associated with the model parameters and the appropriate model structure. These uncertainties may be reduced by comparing the model predictions to measurements using inverse modeling, resulting in posterior parameter distributions that are conditioned on the data used in the calibration. We present the calibration of a regional distributed subsurface water flow model for a 1,400 km2 irrigated agricultural area in the western San Joaquin Valley of California. Two global optimization algorithms were used to identify optimal parameter values and their uncertainties using data on spatially distributed local water table depth measurements, district-average groundwater pumping and district-average subsurface drainage data. Using the single objective function approach, the three measurement types were weighted into a single objective function for global optimization purposes. Additionally, a three-objective multi-criteria optimization problem was formulated in which no prior weighting of the individual objectives was specified. The single-objective optimization approach resulted in identifiable parameters with relatively small uncertainties, however, most likely values for various optimized parameter approached the outer bounds of their physical-realistic ranges. In the multi-objective approach, the objective function of each measurement type was treated independently, so that no subjective preferences were assigned a priori. The estimated Pareto set exhibited large parameter uncertainty, indicating possible model structural inadequacies.

Schoups, G., C. A, Young, J. Vrugt, J. W. Hopmans, and W. W. Wallender (2002). **Estimating vadose zone hydraulic properties of tile-drained fields using inverse modeling.** *Eos Trans. AGU, 83(47), Fall Meet. Suppl., Abstract H12A-0914.*

The prediction of water flow and solute transport through the vadose zone requires knowledge of the spatial distribution of soil hydraulic properties, such as the conductivity and retention parameters. Several point-scale techniques are available for measuring soil hydraulic properties. However, in applications at the field to regional scale, a prohibitively large number of sampling sites are needed to characterize the vadose zone. An alternative approach is to estimate effective values for the hydraulic parameters by inverse modeling. In this study, the inverse approach is applied to a 9600-acres irrigation district located in the San Joaquin Valley, California. The area consists of a number of tile-drained fields for which weekly drain flows are available. A numerical model is used to simulate three-dimensional variably-saturated subsurface water flow as well as field-scale and district-scale drain flows. Input data include spatially distributed crop types and weekly evapotranspiration and irrigation amounts for each field in the district. An inverse algorithm is then applied for optimization to observed drain flows. Optimization parameters are the soil hydraulic parameters, described here by a single spatially distributed scaling factor, and the drain conductances.

Tsou, Ming-Shu, Kan Tu, Jan Kool, Christopher J. Neville, and Steven C. Young, 2003. **Comparison of Three Numerical Models for Chain-Decay Transport Simulation at a Closed AFB in Texas.** *Proceedings MODFLOW 2003 Conference, Golden, Colorado, September 17-19. V.1, pp. 423-427.*

Numerical schemes of three codes, MODFLOW-SURFACT, MT3D99, and RT3D, were compared for simulation of chain decay of PCE at a decommissioned Air Force Base in central Texas, to explore the implications of simulation code and solution scheme selection. The flow field generated by MODFLOWSURFACT was used by MT3D99 and RT3D for transport simulation. Nine different transport models were developed incorporating three solution methods in combination with different time-stepping schemes. The solution methods examined within MODFLOW-SURFACT were TVD/Crank-Nicolson, upstream finite difference/ Crank-Nicolson and upstream finite-difference/fully implicit-in-time weighting. Upstream weighting and fully implicit finite-difference schemes were used for inter-code comparisons. The results obtained with MT3D99 were closer to MODFLOW-SURFACT than to RT3D. RT3D incorporates the implicit assumption that decay reactions occur only in the dissolved phase so it predicts slower overall degradation. The results of the sensitivity analysis confirm that MODFLOW-SURFACT is capable of reproducing results obtained with public-domain transport simulators, and offers increased flexibility in the use of solution methods and time-stepping schemes.

Tu Kan, Jan Kool, Varut Guvanasen, and Ming-Shu Tsou, **Assessment of LNAPL Source Zone and Impacts on Longevity of Dissolved Phase Benzene Plume,** *MODFLOW and More 2006 Managing Groundwater Systems – Conference, Golden, CO., 2006. V.2, p.629.*

This paper presents a case study of a large jet fuel spill site ST012 at former William Air Force Base (WAFB). The total spill volume is estimated to be as high as 1.4 million gallons. Due to fluctuating water table elevations, much of the LNAPL is present in a smear zone, making free product recovery difficult. On the other hand, more than 10 years of monitoring data indicates that the dissolved phase plume is relatively small and stable. A numerical flow and transport model, based on the MODFLOW-SURFACT code (HGL, 2002), was developed to help define and prioritize risk-based site management options. Benzene was selected as the primary constituent of concern. The model represented the LNAPL as a spatially distributed non aqueous source term and accounted for benzene dissolution, source depletion, and transport and natural attenuation in groundwater. The observed stability of the groundwater plume indicates that fuel residual release and mass removal via natural attenuation are approximately balanced. Modeling the source release based on equilibrium partitioning of benzene between the LNAPL and aqueous phases, and using benzene degradation constants estimated from groundwater natural attenuation indicators, resulted in a good match between the simulated and observed groundwater benzene plumes. This result also supported a total LNAPL volume towards the lower range of existing estimates.

Vrugt, J. A., G. Schoups, J. W. Hopmans, C. A. Young, W. W. Wallender, T. H. Harter, and W. Bouten (2003).
I**dentification of spatially distributed soil hydraulic properties in hydrologic modeling using global optimization.** *Eos Trans. AGU, 84(46), Fall Meet. Suppl., Abstract H11I-03.*

In the past few years, computational capabilities have evolved to a point, where it is possible to use multi-dimensional physically based hydrologic models to study spatial and temporal patterns of water flow in the vadose zone. However, so far these models based on complex multi-dimensional governing equations have only received very limited attention, in particular because of their computational, distributed input and parameter estimation requirements. The aim of the present paper is to explore the usefulness and applicability of the inverse method to estimate spatially distributed soil hydraulic properties using the solution of a physically-based three-dimensional distributed model combined with spatially distributed measured tile drainage data from the 4000 ha BWD (BWD) in the San Joaquin Valley of California. The inverse problem is posed within a single criterion Bayesian framework and solved by means of the computerized Shuffled Complex Evolution Metropolis (SCEM-UA) global optimization algorithm. To study the benefits of using a complex spatially distributed three-dimensional vadose zone model, the results of the 3D model were compared with those obtained using a simple conceptual bucket model and a spatially-averaged one-dimensional unsaturated water flow model. District-wide results demonstrate that measured spatially distributed patterns of drainage data contain only limited information towards the identification of the vadose zone model parameters, and are particularly inadequate to identify the soil hydraulic properties. In contrast, the drain conductance, and a bypass coefficient were highly identifiable, indicating that the dominant hydrology of the BWD was determined by drain system properties and preferential flow. Despite the significant CPU time needed for model calibration, results indicate that there are advantages of using physically-based hydrologic models to study spatial and temporal patterns of water flow at the scale of a watershed, as these models not only generate consistent forecasts of spatially-distributed drainage data during the calibration and validation period, but also possess unbiased predictive capabilities of measured groundwater table depths not included in the calibration.

Vrugt, J. A., G. Schoups, J. W. Hopmans, C. A. Young, W. W. Wallender, T. H. Harter, and W. Bouten (2004). **Inverse modeling of large-scale spatially-distributed vadose zone properties using global optimization,** *Water Resources Research, doi:10.1029/2003WR002706.*

Computational capabilities have evolved to a point where it is possible to use multidimensional physically based hydrologic models to study spatial and temporal patterns of water flow in the vadose zone. However, models based on multidimensional governing equations have only received limited attention, in particular because of their computational, distributed input, and parameter estimation requirements. The aim of the present paper is to explore the usefulness and applicability of the inverse method to estimate vadose zone properties using the solution of a physically based, distributed three-dimensional model combined with spatially distributed measured tile drainage data from the 3880-ha BroadviewWater District (BWD) in the San Joaquin Valley of California. The inverse problem is posed within a single-criterion Bayesian framework and solved by means of the computerized Shuffled Complex Evolution Metropolis global optimization algorithm. To study the benefits of using a spatially distributed three-dimensional vadose zone model, the results of the 3-D model were compared with those obtained using a simple storage-based bucket model and a spatially averaged one-dimensional unsaturated water flow model for a 2-year period. District-wide results demonstrate that measured spatially distributed patterns of drainage data contain only limited information for the identification of vadose zone model parameters and are particularly inadequate to identify the soil hydraulic properties. In contrast, the drain conductance and a soil matrix bypass coefficient were well determined, indicating that the dominant hydrology of the BWD was determined by drain system properties and preferential flow. Despite the significant CPU time needed for model calibration, results suggest that there are advantages in using physically based hydrologic models to study spatial and temporal patterns of water flow at the scale of a watershed. These models not only generate consistent forecasts of spatially distributed drainage data during the calibration and validation period but also possess unbiased predictive capabilities with respect to measured groundwater table depths not included in the calibration.

Wei, X., V. Guvanasen, M-S. Tsou (2009). **Uncertainty Analysis of a Regional Groundwater Model.** *The 7th Model CARE 2009 conference. Wuhan, China. September 20th—23rd, 2009*

With the increasing urbanization and population growth, best management of water resources has been an important issue in recent years. Groundwater flow and transport model is an effective tool to aid this decision-making process. To develop a model, one of the most important issues is model calibration and assessment of its uncertainty. This paper presents the uncertainty analysis of a regional groundwater flow and transport model developed for a water resource evaluation project. Sensitivity analysis was performed upon major uncertain model parameters including recharge, hydraulic conductivity, leakances, etc. Through sensitivity analysis, we found the model was most sensitive to recharge, horizontal hydraulic conductivity (K) and vertical leakance. Based on data availability and model sensitivity, we generated random fields and conducted Monte Carlo simulations to determine the model uncertainty associated with horizontal hydraulic conductivity. The Monte Carlo simulation demonstrated that model head prediction uncertainties were likely to occur at locations with larger K heterogeneities and/or higher head gradients but not at locations with high K uncertainties.

Werner, A.D., Gallagher, M.R., Weeks, S.W. 2006. **Regional-scale, fully coupled modelling of stream–aquifer interaction in a tropical catchment,** *Journal of Hydrology, 328(3-4), 497-510.*

The planning and management of water resources in the Pioneer Valley, north-eastern Australia requires a tool for assessing the impact of groundwater and stream abstractions on water supply reliabilities and environmental flows in Sandy Creek (the main surface water system studied). Consequently, a fully coupled stream–aquifer model has been constructed using the code MODHMS, calibrated to near-stream observations of watertable behaviour and multiple components of gauged stream flow. This model has been tested using other methods of estimation, including stream depletion analysis and radon isotope tracer sampling. The coarseness of spatial discretisation, which is required for practical reasons of computational efficiency, limits the model's capacity to simulate small-scale processes (e.g., near-stream groundwater pumping, bank storage effects), and alternative approaches are required to complement the model's range of applicability.

Model predictions of groundwater influx to Sandy Creek are compared with baseflow estimates from three different hydrograph separation techniques, which were found to be unable to reflect the dynamics of Sandy Creek stream–aquifer interactions. The model was also used to infer changes in the water balance of the system caused by historical land use change. This led to constraints on the recharge distribution which can be implemented to improve model calibration performance.

Werner, A.D., Gallagher, M.R. 2006. **Characterisation of sea-water intrusion in the Pioneer Valley, Australia using hydrochemistry and three-dimensional numerical modelling,** *Hydrogeology Journal, DOI 10.1007/s10040-006-0059-7.*

Sea-water intrusion is actively contaminating fresh groundwater reserves in the coastal aquifers of the Pioneer Valley, north-eastern Australia. A three-dimensional sea-water intrusion model has been developed using the MODHMS code to explore regional-scale processes and to aid assessment of management strategies for the system. A sea-water intrusion potential map, produced through analyses of the hydrochemistry, hydrology and hydrogeology, offsets model limitations by providing an alternative appraisal of susceptibility. Sea-water intrusion in the Pioneer Valley is not in equilibrium, and a potential exists for further landward shifts in the extent of saline groundwater. The model required consideration of tidal over-height (the additional hydraulic head at the coast produced by the action of tides), with over-height values in the range 0.5–0.9 m giving improved water-table predictions. The effect of the initial water-table condition dominated the sensitivity of the model to changes in the coastal hydraulic boundary condition. Several salination processes are probably occurring in the Pioneer Valley, rather than just simple landward sea-water advancement from "modern" sources of marine salts. The method of vertical discretisation (i.e. model-layer subdivision) was shown to introduce some errors in the prediction of watertable behaviour.

Young Chuck, Wesley Wallender, Gerrit Schoups, Graham Fogg, Sorab Panday, Jan Hopmans, Thomas Harter, Ted Hsiao, Ken Tanji, Kristen Ward, Richard Howitt, 2007. **Modeling Shallow Water Table Evaporation in Irrigated Regions,** *Irrigation and Drainage Systems, 21(2), 119-132*.

Groundwater discharge through evaporation due to a shallow water table can be an important component of a regional scale water balance. Modeling this phenomenon in irrigated regions where soil moisture varies on short time scales is most accurately accomplished using variably saturated modeling codes. However, the computational demands of these models limit their application to field scale problems. The MODFLOW groundwater modeling code is applicable to regional scale problems and it has an evapotranspiration package that can be used to estimate this form of discharge, however, the use of time-invariant parameters in this module result in evaporation rates that are a function of water table depth only. This paper presents a calibration and validation of the previously developed MOD-HMS model code using lysimeter data. The model is then used to illustrate the dependence of bare soil evaporation rates on water table depth and soil moisture conditions. Finally, an approach for estimating the time varying parameters for the MODFLOW evapotranspiration package using a 1-D variably saturated MOD-HMS model is presented.