EARTH SYSTEMS MODELING IN THE BRAZOS RIVER ALLUVIUM AQUIFER: IMPROVEMENT OF COMPUTATIONAL METHODS AND DEVELOPMENT OF CONCEPTUAL MODEL

A Thesis

by

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ABSTRACT

Traditional hydrologic modeling has compartmentalized the water cycle into distinct components (e.g. rainfall-runoff, river routing, or groundwater flow models). In river valley alluvium aquifers, these processes are too interconnected to be represented accurately by separate models. An integrated modeling framework assesses two or more of these components simultaneously, reducing the error associated with approximated boundary conditions. One integrated model, ParFlow.CLM, offers the advantage of parallel computing, but it lacks any mechanism for incorporating time-varying streamflow as an upstream boundary condition. Previous studies have been limited to headwater catchments. Here, a generalized method is developed for applying transient streamflow at an upstream boundary in ParFlow.CLM.

The upstream inflow method was successfully tested on two domains – one idealized domain with a straight channel, and one small stream catchment in the Brazos River Basin. The stream in the second domain is gaged at the upstream and downstream boundaries. Both tests assumed a homogeneous subsurface, so that the efficacy of the transient streamflow method could be evaluated with minimal complications by groundwater interactions.

Additionally, an integrated conceptual model is presented for the Brazos River Alluvium Aquifer (BRAA), the Brazos River, and the overlying terrain. The BRAA is a floodplain aquifer in central to southeast Texas. This aquifer is highly connected to the Brazos River and experiences localized semi-confined conditions beneath thick surface

clay layers. The conceptual model is designed to be implemented in an Earth system modeling framework and is limited to the central portion of the aquifer in Brazos and Burleson Counties, Texas. Unlike previous models in ParFlow.CLM, this is a high-order subbasin with large inflows from upstream. Additionally, the model incorporates no-flow, transient head, and free drainage boundaries. Preliminary tests suggest the need for a long spin-up period. Long-term simulations will require calibration of surface and subsurface parameters before using the model to assess system behavior.

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NOMENCLATURE

CLM	Common Land Model
Q	Volumetric flow rate [L^3T^{-1}]
A	Cross-sectional area of flow [L^2]
t	Time [T]
β	Momentum correction factor [-]
v	Average velocity over a cross-section [LT^{-1}]
y	Flow depth [L]
g	Acceleration due to gravity [LT^{-2}]
S_0	Channel bottom slope [-]
S_f	Friction slope [-]
S	Saturation [-]
S_s	Specific storage coefficient used in ParFlow [L^{-1}]
ϕ	Porosity [-]
ψ	Pressure head [L]
ρ	Density of water [ML^{-3}]
K	Hydraulic conductivity [LT^{-1}]
k_n	Unit conversion factor [1 $m^{1/3}s^{-1}$ = 1.486 $ft^{1/3}s^{-1}$]
n_M	Manning's roughness coefficient [-]
P_{wet}	Wetted perimeter [L]
$q_{CLM}(i,j,t)$	Precipitation value in CLM forcing data [LT^{-1}]
i_{inlet}	X-coordinate(s) of stream cell(s) on upstream boundary

j_{inlet}	Y-coordinate(s) of stream cell(s) on upstream boundary
$q_{rain}(t)$	Rainfall intensity [LT^{-1}]
$Q_{inlet}(t)$	Streamflow at upstream boundary [L^3T^{-1}]
A_{inlet}	Surface area of grid cell(s) at which upstream flow is applied [L^2]
I	Inflow to stream reach [L^3T^{-1}]
O	Outflow from stream reach [L^3T^{-1}]
K_{mc}	Travel time parameter for Muskingum-Cunge routing [T]
X_{mc}	Weighting factor for Muskingum-Cunge routing [-]
L	Length of reach [L]
T	Top width of water surface [L]
CN	Curve number [in^{-1}]
A_w	Watershed area [L^2]
P	Precipitation [L]
Q_{CN}	Incremental runoff [L^3]
FM-60	Farm to Market Road 60
SH-21	Texas State Highway 21
SH-105	Texas State Highway 105
TWO	Texas Water Observatory
BRAA	Brazos River Alluvium Aquifer
TWDB	Texas Water Development Board
MCL	Maximum contaminant level
GAM	Groundwater availability model

x_{BC}	Location on Navasota river boundary [L]
$H_{BC}(x,t)$	Specified head for boundary condition [L]
$H_{gage}(t)$	Water surface elevation of Brazos River at SH-105 [L]
$H_{Navasota}(x_{BC},t_0)$	Elevation in Navasota River on digital elevation map [L]
$H_{gage}(t_0)$	Elevation at stream gage location on digital elevation map [L]
H_i	Period-averaged head at SH-105 gage for period i [L]
K_{eff}	Effective saturated hydraulic conductivity [LT^{-1}]
k_i	Saturated hydraulic conductivity of layer i [LT^{-1}]
b_i	Vertical thickness of layer i [L]
$T_{modeled}$	Transmissivity in geology model [L^2T^{-1}]
$T_{measured}$	Transmissivity from borehole data [L^2T^{-1}]
RMSE	Root mean squared error

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CHAPTER I

INTRODUCTION AND LITERATURE REVIEW

The interactions between groundwater and surface water are a critical component of the hydrologic cycle, but they have historically been simplified or even ignored in models and planning processes. In Texas, water resources are assessed within a statewide planning and management framework, but groundwater planning strategies are mostly disconnected from surface water allocations (Wurbs 1995).

Many modeling systems have been developed in the last half-century for conventional applications in hydrologic science and engineering. A range of programs are available to simulate surface water hydrology, land-surface evapotranspiration, groundwater flow, or reactive contaminant transport. However, because traditional models focus on a single segment of the water cycle, they require simplified representations of the interface with other processes. For example, a groundwater model may represent a stream as a constant-head boundary. Even if the stream stage changes with time, it is only an input to the model, so the boundary condition is not affected by feedback from the groundwater system (Anderson et al. 2015). Freeze and Harlan (1969) presented a conceptual model for representing these hydrological processes in a single distributed model, in which components would be linked by continuity of mass and momentum, but the concept was not developed for several decades. Now, several integrated surface-subsurface hydrological models are available, which solve shallow overland flow and subsurface flow equations simultaneously in either two or three dimensions (Maxwell et al. 2014).

Groundwater-Surface Water Interactions

From a high-level perspective, fluxes between a stream and aquifer manifest as baseflow in gaining streams or as aquifer recharge from losing streams. On shorter timescales, floods may induce bank storage, or riparian vegetation may cause seasonal localized drawdown (Boufadel and Peridier 2002; Winter 1998). Interactions are particularly important in streams with beds of highly permeable media (as opposed to those flowing directly over basement rock). In such cases, a hyporheic zone develops, in which groundwater and surface water mix. The hyporheic zone often hosts rich biodiversity and facilitates many ecological and hydrologic functions (Hancock 2002). Within this zone, water often flows either from stream to aquifer (recharge) or aquifer to stream (discharge or baseflow), but many other flow configurations can occur, including parallel flow and flow-through (Winter 1998; Woessner 2000). Losing streams may discharge through the subsurface via infiltration or preferential flow paths, either as saturated flow directly into the aquifer or as unsaturated flow in the case of a “detached” aquifer (Winter 1998). Alluvial aquifer systems, which are often closely associated with a river system, are excellent opportunities for using integrated models to examine the hydrologic exchanges and ecosystem functions in the hyporheic zone.

Conventional Methods and Analytical Models

In uncoupled models, the interaction of groundwater and surface water may be represented by a simple approximation of baseflow or channel loss, based on a constant groundwater head (HEC 2016) or loss factors (Wurbs 2011). Real-time monitoring of baseflow is difficult, so estimates may be based on historical surveys such as gain/loss studies, which determine which sections of a stream channel are receiving baseflow from groundwater and which are discharging to the subsurface. Exchange flux volumes can be estimated with several methods, including traditional hydrograph separation, differential gauging, hydraulic gradient analysis (applying Darcy's law), and a mass balance method or chemical hydrograph separation using conservative tracers (e.g. Kendall and McDonnell 2012; Miller et al. 2015; SKM 2012).

Numerical Models

"Coupled" or "integrated" models solve surface and subsurface systems simultaneously, such that the solutions to the Saint Venant equations and the Richards' equation maintain continuity of flux across the surface-subsurface interface (Maxwell et al. 2014). Refsgaard et al. (1998) argue that the integration of models can reduce uncertainty in spite of increased complexity because (a) "internal boundaries are simulated [dynamically]" rather than estimated by the modeler, and (b) more datasets are used in validation of a coupled model than in a single model. In other words, an integrated model can consider and predict multiple output variables (soil moisture, groundwater levels, exchange flux and directions, river stage, salinity, etc.), so any of those can be validated against field data. Available models use one of a few coupling methods. Many depend on the conductance concept, which defines a theoretical interface layer separating surface and subsurface storages (e.g. Panday and Huyakorn 2004; VanderKwaak and Loague 2001). This concept permits the pressures simulated by the Richards' equation model and the Saint Venant equations to differ, and the rate of exchange (infiltration or seepage) is dependent on the difference in the modeled pressures (Anderson et al. 2015; Kollet and Maxwell 2006).

Coupled models are valuable when modeling highly connected domains, such as a stream-aquifer interface, as they replace user-input boundary conditions with dynamically simulated conditions while also simulating feedback processes between the surface and subsurface. Additionally, they are useful for quantifying whether hypothesized processes (e.g. redox changes, clogging) are actually occurring to such a degree that hydrologic and/or ecological functions are being affected (Refsgaard et al. 1998).

In the past decade, the USGS has developed coupled models to account for surface water interactions: GSFLOW (coupled to the USGS Precipitation-Runoff Modeling System), SWR (simulates surface-water routing and interactions with groundwater), and MODFLOW-OWHM (the One Water Hydrologic Flow Model for supply-and-demand analysis) (USGS 2016b). These and other currently available integrated models are listed in Table 1 (De Maet et al. 2015; Maxwell et al. 2014; Sebben et al. 2013; Shi et al. 2013; VanderKwaak and Loague 2001). One model, ParFlow, was first developed to utilize parallel computing for the modeling of groundwater flow (Ashby and Falgout 1996). An overland flow simulator was later coupled to the system, incorporating the kinematic wave routing method and a pressure continuity condition at the surface-subsurface interface (Kollet and Maxwell 2006). Unlike the conductance concept used in previous models, the pressure continuity condition forces surface and subsurface pressures to match exactly, which eliminates the need for parameterization of the interface layer (Kollet and Maxwell 2006). The program tested well for computational scalability early in its development, and parallel computing efficiency was acceptable for large model domains (Kollet and Maxwell 2006). Land surface processes can be also modeled in ParFlow.CLM, in which a version of the Common Land Model has been integrated with the overland flow and subsurface model (Kollet and Maxwell 2008; Maxwell and Miller 2005).

Table 1. Integrated surface-subsurface hydrological models

Model Name	Parallel Computing	Vadose Zone Flow	Groundwater Flow	Overland Flow	Evapo-transpiration
CATHY	No	Yes	Yes	Yes	n/a
deMaet et al 2015	No*	Yes	Yes	Yes	No
FIHM / PIHM / Flux-PIHM*	No	Yes	Yes	Yes	Yes
HydroGeoSphere	Yes	Yes	Yes	Yes	Yes
InHm (Integrated Hydrology Model)	No	Yes	Yes	Yes	No*
MODHMS	n/a	n/a	Yes	Yes	Yes
OpenGeoSys	No	Yes	Yes	Yes	n/a
ParFlow	Yes	Yes	Yes	Yes	Yes
PAWS	No	Yes	Yes	Yes	n/a
tRIBS-VEGGIE	No	Yes	Yes	Yes	Yes
GSFLOW	No	Yes	Yes	Yes	Yes
MODFLOW-OWHM	No	Yes	Yes	Yes	Yes
SWR	No	n/a	Yes	Yes	n/a

CHAPTER II

METHOD FOR MODELING HIGH-TEMPORAL-RESOLUTION STREAM INFLOWS IN A LONG-TERM PARFLOW.CLM SIMULATION

Introduction

ParFlow.CLM is a powerful tool for large-scale Earth systems modeling. Its surface – subsurface coupling makes it preferable to MODFLOW for shallow alluvial aquifers that may interact significantly with surface streams. The inclusion of the land surface model CLM permits a highly complex simulation of the water cycle within the critical zone. Additionally, ParFlow.CLM has the advantage of parallelization, allowing large domains to be run at acceptable resolutions on multiple processors at a time. Several integrated hydrological models are available (e.g. ParFlow (Ashby and Falgout 1996; Kollet and Maxwell 2006), InHm (VanderKwaak and Loague 2001), MODHMS (Panday and Huyakorn 2004), and HydroGeoSphere (Hwang et al. 2014)), but parallelization among integrated surface-subsurface hydrological models is unique to ParFlow and HydroGeoSphere (Maxwell et al. 2014).

Simulations using ParFlow and ParFlow.CLM have included small and large domains, from idealized boxes to real heterogeneous watersheds, and have assessed computational efficiency, spin-up behavior, parameter sensitivity, and even the development of a continental-scale groundwater model for the contiguous United States (Ajami et al. 2015; Ajami et al. 2014; Kollet et al. 2010; Maxwell et al. 2015; Seck et al. 2015; Srivastava et al. 2014). However, almost all of the published studies include the headwaters for any streams within the domain, so any streamflow in the domain is generated by groundwater contributions and precipitation runoff. The exception is an assessment of stream-aquifer interactions by Frei et al. (2009), which used ParFlow (not coupled to CLM) to simulate flow in a heterogeneous box domain with a straight, rectangular channel over a 30-day period with daily stress periods.

In its present state, ParFlow.CLM does not have the capability to include stream inflow as a transient boundary condition. When a Dirichlet boundary condition has a specified head greater than the land surface elevation, surface flow is generated automatically. However, this means that a boundary containing a stream must have a specified-head (Dirichlet) condition rather than a specified-flow (Neumann) condition. For situations in which groundwater flow is primarily toward a stream, rather than parallel to the stream, no-flow boundaries are more appropriate and this becomes an important modeling limitation. Additionally, ParFlow does not accept input files to specify a time series of streamflow or boundary head values. Instead, transience in ParFlow is handled with user-specified “cycles” – repeating series of time intervals. Rather than providing a time-series of boundary conditions, well pumping, or streamflow, conditions must remain constant for each period of a defined cycle (Maxwell et al. 2016). This is feasible for simulations with a small total number of timesteps (e.g. Frei et al. (2009)), but it makes transient boundary conditions difficult to set up for a long-term simulation. Previous long-term ParFlow simulations have modeled the domain from headwater to outlet (Condon et al. 2013; Engdahl and Maxwell 2015; Schalge et al. 2016; Srivastava et al. 2014), so transient upstream inflows have not been required.

Considering this shortcoming, this project sought to develop a general method for introducing transient streamflow over long time periods at high temporal resolution (e.g. hourly flow for multiple months). Implementing file-based streamflow input would expand the applicability of the modeling system to a more generalized set of domains.

The objectives of this thesis are to:

1. Develop a reliable method for generating transient surface flow in ParFlow.
2. Present a workflow for applying this method in a long-term simulation at a fine temporal resolution.
3. Summarize method usability: ease of convergence, spin-up time, and computational efficiency.
4. Prove viability of method for multiple domains (one synthetic catchment and one idealized real catchment).
5. Demonstrate the effect of a coupled subsurface model on surface flow hydrographs by comparing modeled outflow hydrographs to predictions by traditional routing methodologies.
6. Illustrate subsurface hydraulic response during a flood pulse.

Background

Governing Equations

Overland flows are governed by the Saint Venant equations (Akan 2006), which describe conservation of mass (Equation 1) and conservation of momentum (Equation 2).

$$\frac{\delta A}{\delta t} + \frac{\delta Q}{\delta x} = 0 \qquad \text{Equation 1}$$

$$\frac{\delta Q}{\delta t} + \frac{\delta}{\delta x}(\beta Q v) + gA\frac{\delta y}{\delta x} + gAS_f - gAS_0 = 0 \qquad \text{Equation 2}$$

In both of these, x is positive displacement in the direction of downstream flow [L], t is time [T], Q is the volumetric flow rate [L^3T^{-1}], and A is the cross-sectional flow area [L^2]. Additionally, the momentum equation considers gravitational acceleration g [LT^{-2}], a momentum correction factor β [-], average velocity over a cross-section v [LT^{-1}], flow depth y [L], friction slope S_f [-], and channel bed slope S_0 [-].

Although uncoupled models typically rely on Darcy's equation for fully-saturated flow through porous media, Darcy's law is insufficient for coupled models, which need to accurately represent the unsaturated vadose zone between the groundwater table and the land surface. Richards' partial differential equation relates saturation, matric potential (or pressure head, ψ [L]), the density of water ρ [ML^{-3}], and hydraulic conductivity K [LT^{-1}] to describes flow in variably-saturated porous media, in which water is under tension and governed by capillary forces. Shown in Equation 3 is Richards' equation as it is implemented in ParFlow (Maxwell et al. 2016), in which S is saturation [-], ψ is pressure head [L], S_s is a specific storage coefficient [L^{-1}], ϕ is porosity [-], ρ is density [ML^{-3}], $\vec{g}$ is acceleration due to gravity [L^2T^{-1}], $\boldsymbol{K}$ is the hydraulic conductivity tensor [LT^{-1}] and Q_s is a source/sink term [L^3T^{-1}].

$$S(\psi)S_s\frac{\delta\psi}{\delta t} = \delta\big(\phi S(\psi)\rho(\psi)\big)\frac{1}{\delta t} + \nabla\cdot\Big(\vec{g}\boldsymbol{K}(\psi)\rho(\psi)\big(\nabla\psi - \rho(\psi)\big)\Big) + Q_s \qquad \text{Equation 3}$$

Porous media properties such as dispersivity and saturated hydraulic conductivity, are typically determined by field assessments, model calibration, or possibly lab tests. These and soil hydraulic parameters based on formulations by van Genuchten (1980) or Brooks and Corey (1964) may be used to determine the hydraulic conductivity for a given pressure head.

ParFlow.CLM

In ParFlow, the St. Venant equation for conservation of momentum is reduced to the kinematic wave approximation (Equation 4), which assumes that diffusion is negligible, such that the friction slope (S_f) and channel slope (S_0) are equal at each point in space. Additionally, Manning's equation (Akan 2006) is used to solve for head losses due to surface roughness (Equation 5).

$$S_0 = S_f \qquad \text{Equation 4}$$

$$Q = \frac{k_n}{n_M} * A^{\frac{5}{3}} * P_{wet}^{-\frac{2}{3}} * S_f^{\frac{1}{2}} \qquad \text{Equation 5}$$

The friction slope S_f describes head loss per unit distance [-]; Q is the volumetric rate of flow [L^3T^{-1}], k_n is a unit conversion factor (1 $m^{1/3}s^{-1}$ = 1.486 $ft^{1/3}s^{-1}$), n_M is Manning's roughness coefficient [-], A is the cross-sectional area of flow [L^2], and P_{wet} is the wetted perimeter of the cross-section [L].

ParFlow accepts four forms of soil hydraulic functions to describe relative permeability as a function of pressure – the van Genuchten relationship, the Haverkamp model, a simple polynomial function, or a constant relative permeability (Maxwell et al. 2016). Similarly, the saturated hydraulic conductivity in a ParFlow domain can be applied as a homogeneous constant, a known value for each grid cell, or a stochastic field using either the turning bands method or a Gaussian simulator (Maxwell et al. 2016).

Details of the numerical discretization and solution methods applied in ParFlow have been described in depth by Huyakorn and Pinder (1983), Jones and Woodward (2001), and Kollet and Maxwell (2006). In short, pressure and saturation in the variably-saturated subsurface are solved based on a discretized form of Richards' equation using a block-centered finite difference model (Kollet and Maxwell 2006). The surface hydrology component is addressed with a finite control volume discretization to solve the continuity equation using the kinematic wave approximation and Manning's equation (Kollet and Maxwell 2006). At each time-step, the surface and subsurface conditions are reconciled by a pressure continuity condition, which requires that "the pressures of the surface and subsurface domains are continuous (equal) right at the land surface," (Kollet and Maxwell 2006, 948). Then, the flux introduced as a boundary condition to the subsurface is the same as the infiltration (or evaporation) flux calculated on the surface.

Methodology

Method Formulation for a Transient Streamflow Boundary Condition

In ParFlow, overland flow is a function of pressure head in the uppermost cells. When pressure in these cells is greater than zero, ponding occurs and overland flow forms. Because surface water is only a function of pressure in the subsurface, it cannot be defined on its own as a boundary condition. However, surface water can be generated by the following methods:

- *Internal Dirichlet boundary condition:* Pressure head is specified at a location in the subsurface. If associated hydraulic head is greater than the land surface elevation above that location, surface flow should form once the pressure in the internal boundary cell has propagated upward.
- *Non-transient rainfall file:* A spatially-heterogeneous 2D file of precipitation over the domain can be applied. If rainfall exceeds the infiltration capacity in a cell, ponding occurs.
- *Boundary pressure equation:* Head along a side of the domain can be specified by a piecewise linear equation (e.g. generating a losing or gaining stream), such that head at the stream cells is greater than land surface elevation.
- *Pressure file boundary condition:* Head along a side of the domain is specified in a 3D file, so the boundary is not necessarily in hydrostatic equilibrium, nor is it limited to a linear water table as with the pressure equation.
- *Injection:* Additional water can be introduced to the domain in any number of cells at a specified input flux.

An internal Dirichlet boundary condition is limited to a constant head value for the entirety of a simulation period. “Injection” must either be constant or a simple pre-defined function of time and location in the domain. The remaining methods are limited temporally to the “cycles” in ParFlow. Table 2 describes the advantages and disadvantages of each method. Of the five methods for simulating steady-state surface flow, the "injection" method was selected as most reliable and most generally applicable. This method can be applied to any cell in the domain, including edge cells. It does not automatically generate surface storage; instead, it functions like an injection well and increases subsurface pressure. To simulate inflow from a stream, water is injected in the uppermost cell of the active domain at the point where the stream crosses the upstream boundary. A spin-up period with a steady-state injection flowrate is necessary to allow subsurface conditions to equilibrate, after which the injection cell functions like a spring and forms a stream.

Table 2. Methods for inducing surface flow in ParFlow

Method	Pros	Cons
Internal boundary condition	Automatically simulates surface water when hydraulic head > land surface elevation	Not applicable on boundary of domain Inconsistent functioning in ParFlow
2D rainfall file	Quickly generates surface flow via infiltration excess Can be applied on edge of domain	Cannot be used simultaneously with CLM
Linear equation for head on boundary	Applied as a ParFlow boundary condition	Cannot specify a no-flow boundary near the inlet
Pressure file	Applied as a ParFlow boundary condition	Cannot specify a no-flow boundary near the inlet May require extensive pre-processing
Injection	Easy to implement	Flux cannot change between defined time cycles

CLM uses file-based inputs instead of the one-at-a-time parameter keys used by ParFlow. Files contain meteorological forcing data for every timestep of the simulation. As with the non-transient rainfall files in ParFlow, ParFlow.CLM forcing data can be spatially distributed, such that surface flow can be applied to a model cell by augmenting the precipitation at that location. In this way, transient streamflow can be applied as forcing data, acting like a boundary condition. Using injection for the steady-state streamflow, rather than CLM forcing data, reduces the volume of input files needed for model spin-up.

Here, a general method is developed to incorporate time-series inflow data at the upstream end of a model domain. The uppermost cell at the upstream end of the channel is referred to as the "inlet." Streamflow at the inlet, $Q_{inlet}(t)$, is first generated by steady-state injection during model initialization. Steady-state flow is set equal to the total inflow at the beginning of the intended simulation period. Once the inlet streamflow has propagated down-channel to the outlet, injection is turned off. Then the long-term transient simulation is begun, during which $Q_{inlet}(t)$ is incorporated as part of the CLM forcing data. Meteorological forcing data can be spatially heterogeneous in CLM, so precipitation flux is modified to include stream inflow only over the grid cell at the inlet location, as shown here:

$$q_{CLM}(i_{inlet}, j_{inlet}, t) = q_{rain}(t) + \frac{Q_{inlet}(t)}{A_{inlet}} \qquad \text{Equation 6}$$

where $q_{CLM}(i, j, t)$ is the flux value in the gridded CLM input file. For every timestep t, gaged streamflow near the inlet, $Q_{inlet}(t)$ [L^3T^{-1}] is converted to an "intensity" value by dividing by the surface area of the grid cell(s) closest to the inlet, A_{inlet} [L^2]. This value is then added to measured rainfall intensity $q_{rain}(t)$ [LT^{-1}] at the inlet grid cell(s), located at (i_{inlet}, j_{inlet}).

Experimental Design

A spin-up and simulation were conducted for each of two model domains, one synthetic case and one based on a real-world setting. The modeling process included initialization of the groundwater conditions and steady-state streamflow, recursive runs with CLM (spin-up), and the simulation of several months of real rainfall and meteorological data. The orthogonal grid formulation was used in ParFlow, but future simulations could test the applicability of the method with the terrain-following grid option (Maxwell 2013).

All model runs were done with parallel processing on 100 computing cores on the high-performance computing cluster "Terra," housed in High Performance Research Computing at Texas A&M University. Terra is a Lenovo cluster with 8,512 cores and a peak performance of 326 teraFLOPS (floating-point operations per second). It has a total 3 PB of raw storage, of which 1 PB is dedicated for use by the Center for Geospatial Science, Applications, and Technology (GEOSAT) and has been made available to this project (TAMU-HPRC 2017).

Synthetic Catchment

Several studies have used a "tilted V catchment" as a test case for evaluating integrated hydrologic models. However, these usually employ a thin or 2-dimensional domain and assess only surface flow (Kollet and Maxwell 2006; Maxwell et al. 2014;

Panday and Huyakorn 2004; Sulis et al. 2010). Here, the tilted V was used as the topography in a 3-dimensional domain – a rectangular domain is sloped inward towards a central channel, then tilted slightly downstream (Figure 1). Dirichlet-type boundaries are specified on the sides parallel to the channel with head values either 1 m above or 1 m below the channel bottom. No-flow boundaries are set on the inlet and outlet sides of the domain and at the bottom. The subsurface is represented as a homogeneous, highly-permeable soil with 60% sand and 15% clay, and vegetation is classified as "grassland" for the entire domain. This geometry provides a simple, idealized domain for easy testing and evaluation.

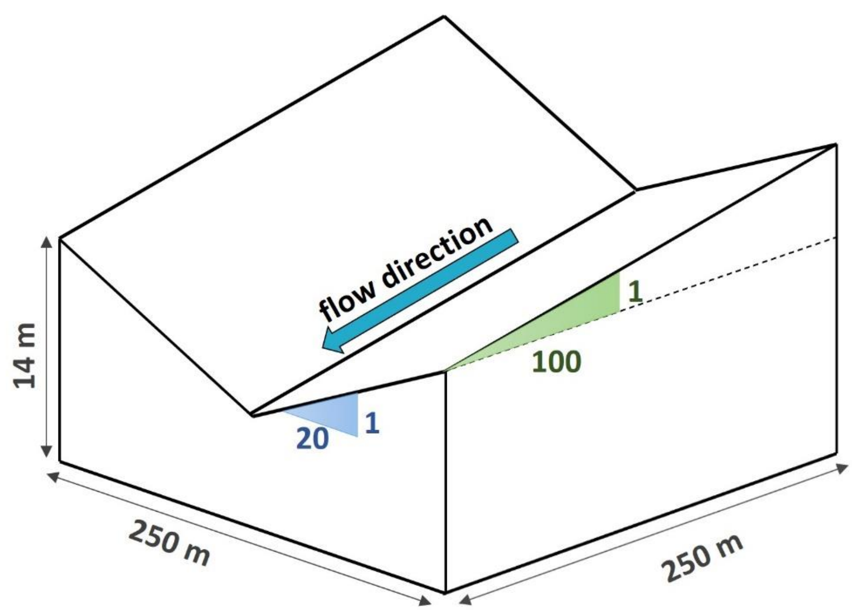

Figure 1. Tilted V catchment

Thompson Creek Catchment

In addition to the tilted V problem, a second model domain is created for the Thompson Creek drainage area, a small catchment in the Brazos River basin near Bryan, TX (Figure 2). The Brazos River cuts through the area, with upstream and downstream boundaries near stream gages at SH-21 and FM-60, respectively (Figure 3). Land surface forcing data are estimated from meteorological data for Easterwood Airport in College Station. Hourly streamflow at the upstream gage has been measured continuously since 1993 (USGS 2016c), and streamflow at the outlet was measured every 20 minutes from September 2015 until February 2016 (personal communication, Kimberly Rhodes, 2016). This catchment provides a good test domain for the introduction of known transient upstream flow, land surface runoff, groundwater interaction, and comparison to a known transient flow at the outlet.

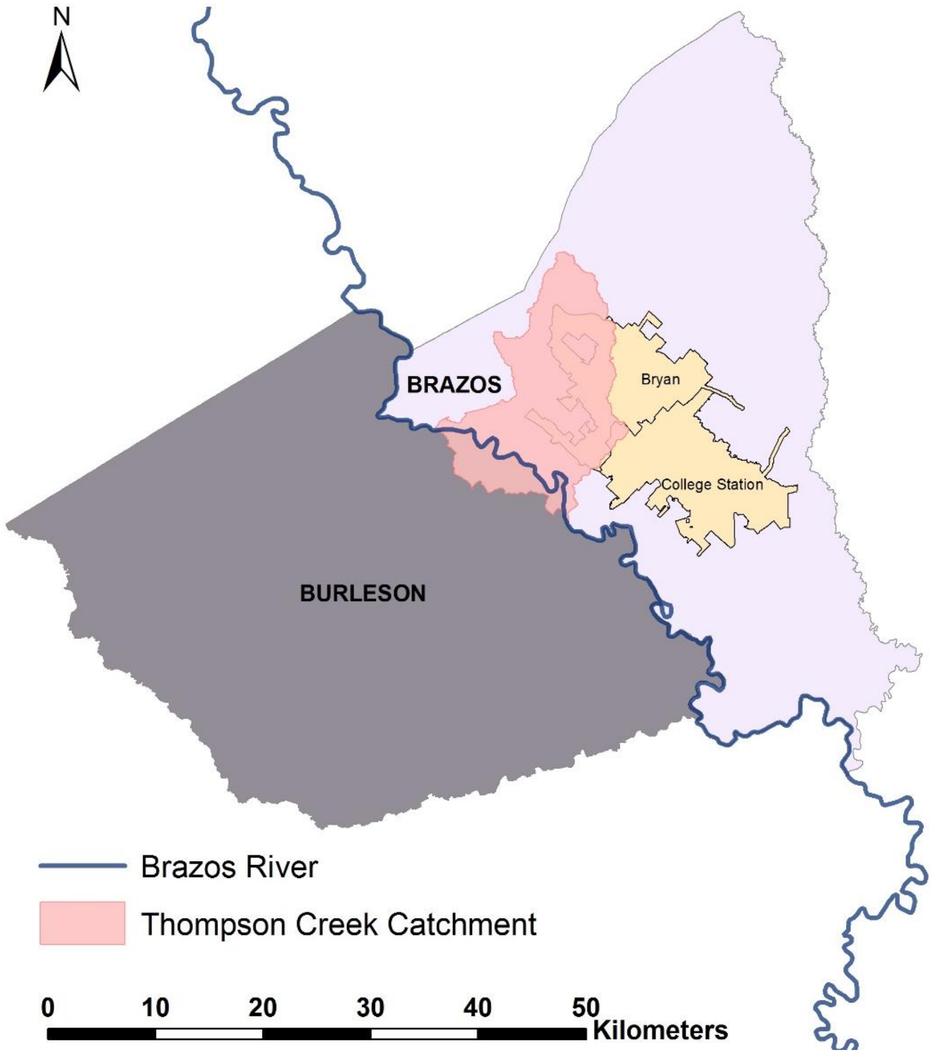

Figure 2. Location of Thompson Creek catchment

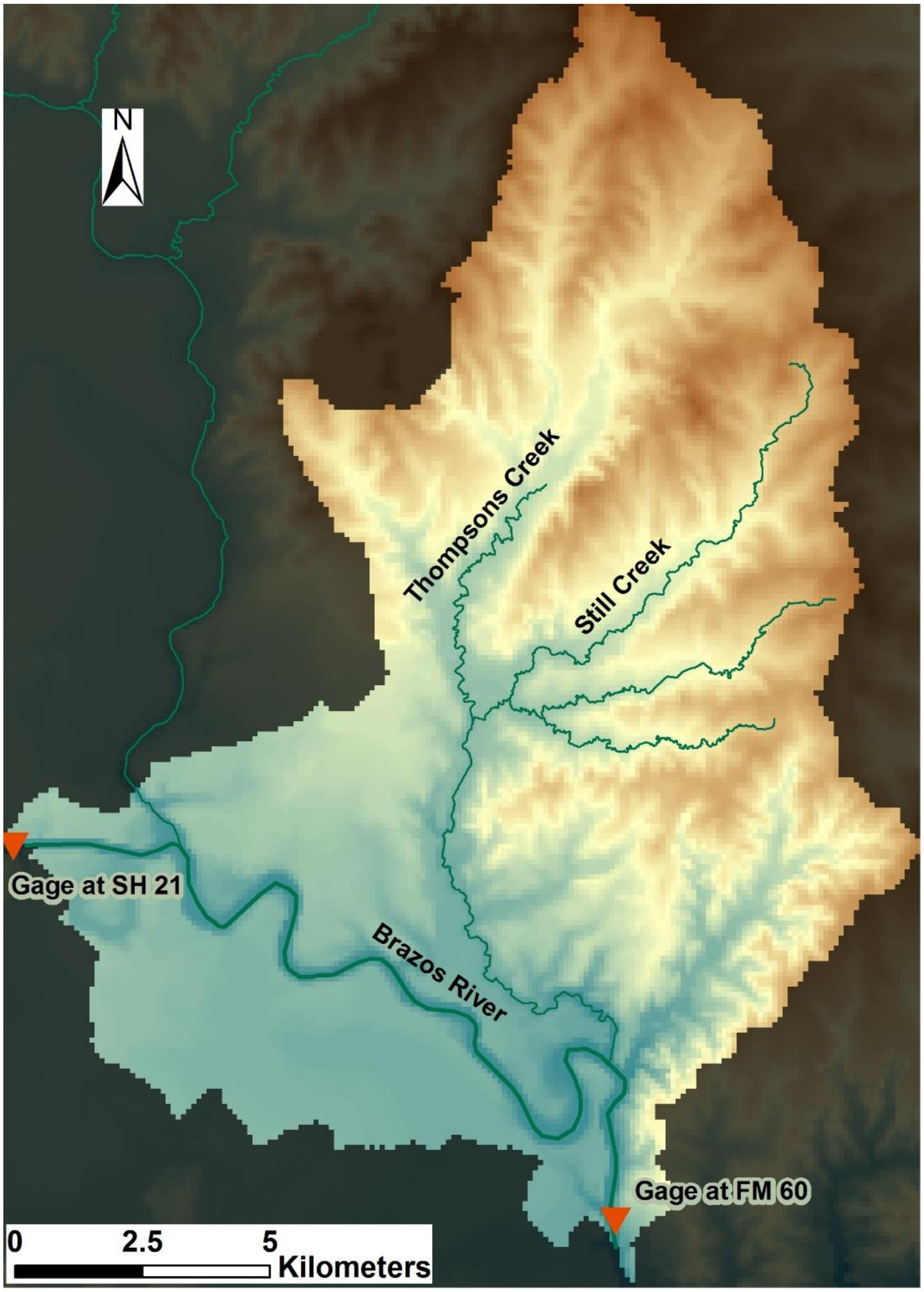

Figure 3. Streams and stream gages in Thompson Creek catchment

The domain boundaries follow watershed divides, but the catchment does include a portion of the Brazos River Alluvium Aquifer. For the purposes of testing the transient streamflow method, groundwater processes were simplified. At the beginning of the spin-up period (October 2014 – October 2015) the groundwater table is initialized at a constant elevation based on a nearby monitoring well measurement from February 2014. The perimeter of the subsurface domain is modeled as a no-flow boundary. Additionally, subsurface properties are the same as those for the tilted V catchment. Hydraulic properties are listed in Table 3.

Table 3. Hydraulic properties for tilted V and Thompson Creek catchments

Parameter	Value
Saturated hydraulic conductivity	1.0 m/hr
Porosity	0.35
$\boldsymbol{\alpha}$, van Genuchten	3.5 m^{-1}
$\boldsymbol{n}$, van Genuchten	3.2
Residual saturation	0.10

Model Spin-Up

Model spin-up refers to running the model with long-term forcing data prior to the simulation period to generate a physically realistic initial state for the intended simulation. This step is important in reducing the impact of the initial condition so that the output is a more accurate representation of the system’s response to forcing data

(Ajami et al. 2015; Ajami et al. 2014; Seck et al. 2015). For this study, a three-phase model initialization scheme was developed which incorporated steady-state streamflow prior to simulating a transient upstream flow boundary condition. All final simulations were done at an hourly timestep; a 0.1-hour timestep was used in the early spin-up phases for the Thompson Creek catchment to improve model convergence.

First, ParFlow was run alone (without CLM) with steady-state boundary conditions. Because ParFlow includes vadose zone and surface runoff processes, average annual rainfall – *not* aquifer recharge – was applied to the land surface at a constant rate. Average rainfall near the Thompson Creek catchment is approximately 1000 mm/year; this value was used for both domains. Streamflow was also initialized during this phase using the injection method at the upstream boundary. The injection flowrate was equivalent to the upstream inflow in the first timestep of the transient simulation period. The cross-sections in Figure 4, taken at the upstream boundary of the tilted V domain, demonstrate the rapid response of the subsurface to injected flux at the stream inlet. A single cell was used for injection, and the large head gradient induced by the added flow rapidly produced surface ponding. Similarly, lateral flow developed and adjacent cells became saturated. For this small domain, the groundwater table at this cross-section had formed a typical losing-stream profile in less than 48 simulation hours. In the second phase, CLM was turned on, and gridded vegetation and soil data were included as inputs. Boundary conditions remained the same except that constant rainfall was applied as part of CLM forcing data.

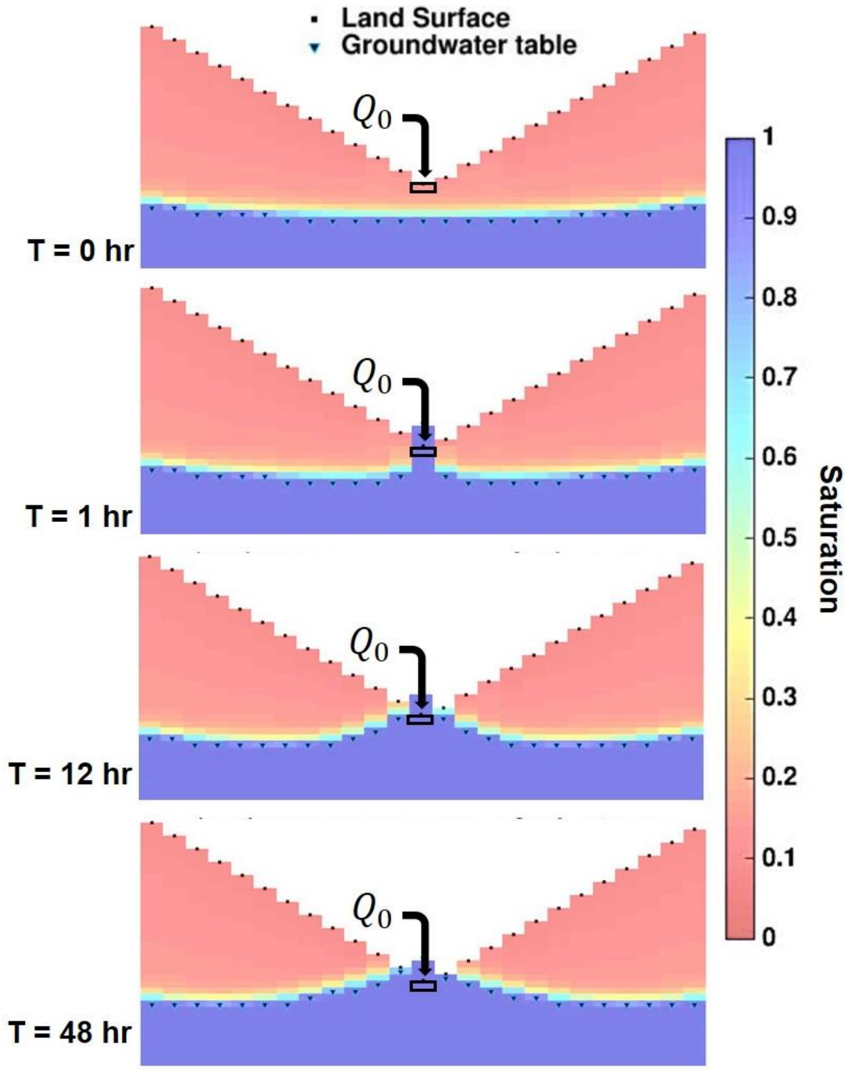

Figure 4. Cross-section of subsurface saturation at upstream boundary during first 48 hours of injection

The objective of the first two phases was to reach an approximate steady state with long-term recharge and constant streamflow, from which model spin-up could continue with transient forcing data. Because the boundary conditions were non-transient, percentage change in storage volumes of groundwater, unsaturated zone, and total domain (subsurface and surface) were assessed every timestep. Ajami et al. (2014) suggested that equilibrium of some criteria "should be considered in terms of stabilization of percent change values rather than via predefined thresholds (2654)." Indeed, stopping at predefined percent change thresholds often did not capture the dynamics of the spin-up cycle. For example, percent changes in total groundwater storage might be very small from the start because most of the groundwater storage pool remains saturated, but spatial distribution of saturated storage near the water table can change significantly during early spin-up. Instead, stabilization of percent changes were evaluated by setting a maximum threshold for the slope of the percent change line (Figure 5). Phases I and II were considered complete when the slope of the percent-change line for each of four state variables (saturated storage, unsaturated storage, runoff at the outlet, and spatially-averaged depth to water table) fell below 0.01.

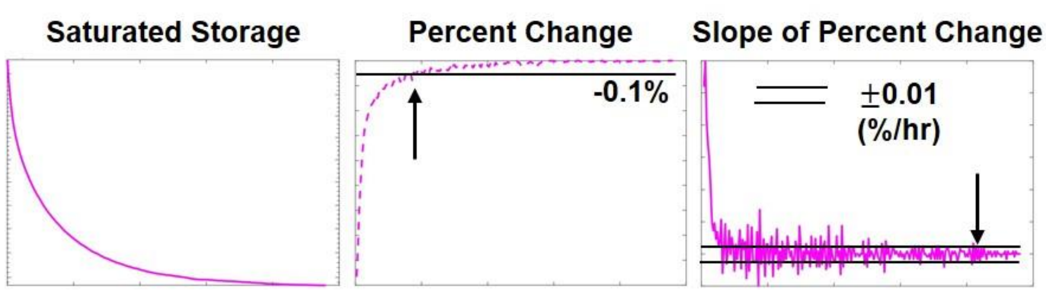

Figure 5. Example time-series of saturated storage during phase I of spin-up (arrows denote times at which percent-cutoff and stabilization threshold values are reached)

After the model state reached an approximate steady state with the constant rainfall, it was run recursively with one year of forcing data. The one-year period prior to the start of each intended simulation was used as the spin-up year. The end state of each recursive run was used as the initial condition for the next, until defined stop criteria were met. Injected upstream flow remained constant during this phase. The one-year simulation was completed at least twice, and recursive runs were evaluated based on year-to-year changes in end-of-year groundwater storage, end-of-year mean depth-to-groundwater (averaged over the domain), end-of-year unsaturated zone storage, and end-of-year surface runoff (discharge at the outlet). For this third phase, stop criteria in the multi-year recursive runs were simple threshold values for percent change in each end-of-year value. The unsaturated zone storage and depth to water table were expected to take the longest to equilibrate, as subsurface equilibrium is more likely to reduce initial condition bias in the final simulation than equilibrium in runoff or energy fluxes (Ajami et al. 2014). However, in previous studies, streamflow at the outlet was limited to runoff from within the domain. Because streamflow in this framework was controlled more directly by the new upstream boundary condition, annual changes in surface runoff were evaluated during spin-up as well.

Routing and Runoff Calculations

Outlet streamflow for the tilted V catchment was calculated separately from the model using the Muskingum-Cunge hydraulic routing method (Akan 2006) and the SCS runoff curve number method (USDA-NRCS 1986). The Muskingum-Cunge method predicts runoff at the outlet of a reach based on upstream inflow and channel characteristics. In each timestep, outflow is calculated using outflow (O_{i-1}) and inflow (I_{i-1}) from the previous timestep and inflow (I_i) in the present timestep:

$$O_i = C_0 I_i + C_1 I_{i-1} + C_2 O_{i-1} \quad \text{Equation 7}$$

$$C_0 = \frac{\frac{\Delta t}{K_{mc}} - 2X_{mc}}{2(1 - X_{mc}) + \Delta t/K_{mc}} \quad \text{Equation 8}$$

$$C_1 = \frac{\frac{\Delta t}{K_{mc}} + 2X_{mc}}{2(1 - X_{mc}) + \Delta t/K_{mc}} \quad \text{Equation 9}$$

$$C_2 = \frac{2(1 - X_{mc}) - \Delta t/K_{mc}}{2(1 - X_{mc}) + \Delta t/K_{mc}} \quad \text{Equation 10}$$

The coefficients C_0, C_1, and C_2 depend on the modeling timestep, reach length, and two parameters, K_{mc} and X_{mc}. The method is based on the Muskingum storage equation used in hydrologic routing, with the addition of more physically-based K_{mc} and X_{mc} parameters.

Reference values for flow rate (Q_{ref}), velocity (v_{ref}), and top channel width (T_{ref}) were calculated using Manning's equation (Equation 5), as described in Akan (2006), using a normal flow depth of 1.0 m. These reference values were used in the calculation of K_{mc} and X_{mc} (Equations 11 and 12), in which S_0 is the channel bed slope and L is the length of the reach.

$$X_{mc} = 0.5 * (1 - \frac{Q_{ref}}{\frac{5}{3} * S_0 * L * T_{ref} * v_{ref}}) \quad \text{Equation 11}$$

$$K_{mc} = \frac{L}{\frac{5}{3} * V_{ref}} \quad \text{Equation 12}$$

The SCS runoff curve number method is frequently used to estimate runoff from a watershed of known area A_w, with an assigned “curve number” (CN) based on soil and vegetation properties. The curve number is also dependent on antecedent moisture conditions, but for these calculations, it was considered constant throughout the simulation. The curve number method estimates runoff at the outlet (Q_{CN} [L^3T^{-1}]) for each time interval (e.g. each hour) of a given storm by

$$Q_{CN} = A_w * \frac{1}{\Delta t} * \frac{\left(P - 0.2 * \left(\frac{1000}{CN} - 10\right)\right)^2}{P + 0.8 * \left(\frac{1000}{CN} - 10\right)} \quad \text{Equation 13}$$

where P is the precipitation depth in inches during time interval Δt. A curve number of 39 was used for the tilted V catchment; this is appropriate for open spaces (e.g. pasture or golf course) with >75% grass cover and a sandy soil (USDA-NRCS 1986), similar to the previously defined properties for this domain.

The Muskingum-Cunge routing method was only applied to the flow introduced at the upstream boundary; runoff predicted by the curve number method was assumed to accumulate at the domain outlet. The outflow hydrographs predicted by Muskingum-Cunge and the curve number method were summed at each timestep to produce a predicted hydrograph, referred to hereafter as the routing/runoff prediction. This calculated hydrograph was compared to the modeled discharge for the synthetic catchment.

Results and Discussion

Tilted V Simulation

Spin-up

A thorough model spin-up was completed in the tilted V catchment for two scenarios. The constant-head boundaries were set so that the regional groundwater table was approximately 1 m below or 1 m above the streambed, simulating either losing-stream or gaining-stream conditions, respectively. The model was run at an hourly timestep. Spin-up times shown in Table 4 refer to the number of days simulated before beginning the next phase for the losing-stream scenario. Steady-state conditions in phase I (ParFlow only) were run for ten days, after which CLM was activated. Phase II was run for one year and then evaluated for stabilization of percent change values. Unsaturated zone storage took the longest to stabilize (287 days for losing stream). The output state of Day 287 was then used as the initial condition for the multi-year recursive runs. Finally, five years of recursive model runs were completed so that all end-of-year criteria reached a percent change of < 0.1%.

As a small, homogeneous domain, this model typically required < 0.01 CPU-hours per model hour during spin-up and an average of 0.013 CPU-hours per model hour during the transient simulation. The total spin-up period (297 days plus 5 years) took 189 CPU-hours to complete. The gaining-stream scenario behaved similarly but reached stop criteria more quickly. Phases I and II were completed in 222 days, and only four spin-up years were required to reach the percent-change thresholds. However, it should be noted that percent changes increased slightly after a fifth spin-up year, suggesting that the year-to-year changes are still fluctuating rather than consistently decreasing. Although the percent-change threshold criteria was met after year 4, it was exceeded again in year 5. Here, model spin-up was considered complete after four years using a strict interpretation of the stop criteria. However, additional spin-up years would be required for state variables to consistently stay below the percent-change threshold.

Table 4. Time to reach spin-up stop criteria in the tilted V catchment under losing-stream conditions

	Spin-up stop times (model days)	S_{GW}	S_{unsat}	Q_{outlet}	$\overline{DTW}$
Phase I (steady-state, ParFlow only)	Percent cutoff time (0.1%)	3.8	9.7	5.0	1.5
	PC-stabilization time	9.75	>10	1.2	>10
Phase II steady-state with CLM)	Percent cutoff time (0.1%)	<1	4.0	1.4	15.3
	PC-stabilization time	5.1	287	1	15.3
Phase III (recursive 1-year runs)	Years to <1%	2	2	2	2
	Years to <0.1%	3	5	5	5

Simulation

Transient stream inflow was applied to the synthetic tilted V catchment for a 10-month period based on data in Burleson County, TX. Hourly forcing inputs were based on temperature, precipitation, solar radiation, and barometric pressure data measured near the Brazos River and FM 60 for January 1 – November 1, 2015 (data from Department of Atmospheric Sciences, TAMU). Stream gage data for the Brazos River at

SH-21 were used for inlet flow (USGS 2016c), but flowrates were reduced by a factor of 50 to suit the small tilted V domain. The synthetic catchment includes a straight, triangular channel, 250 m in length, with homogeneous land cover and subsurface properties. Modeled discharge at the outlet was compared to a hydrograph predicted by routing and runoff calculations. The first month exhibited some numerical instability; otherwise, modeled outflow matched inflow and the routing/runoff prediction very well, as shown Figure 6.

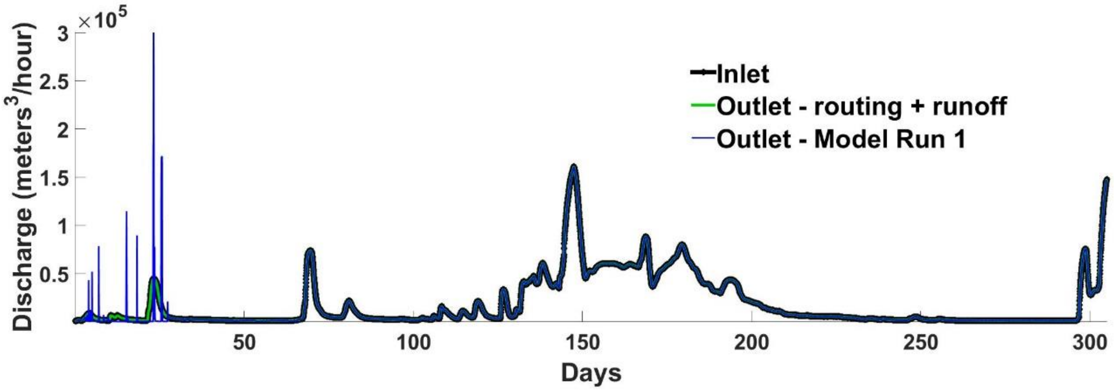

Figure 6. Hydrographs for tilted V catchment

It should be noted that the constant-head boundaries for the synthetic domain are only 120 m from the stream in each direction, so boundary conditions likely have a strong influence on streamflow. This test successfully demonstrated that time-variable streamflow can be introduced to a single “inlet” cell in ParFlow as a transient boundary condition.

Model vs Routing/Runoff Prediction

The hydrographs produced by ParFlow.CLM for each scenario were compared to the routing/runoff prediction (Equations 7 – 13), although an exact match was not expected. Instead, differences represent the improvement afforded by a fully-integrated modeling approach over traditional runoff and routing methods. The discharge predicted by runoff and routing methods is based on surface hydrologic processes, so it does not account for time-variable exchanges between a stream and an aquifer. Thus, a best-fit line of predicted vs modeled discharge can be used to estimate the average gain from or loss to the subsurface, by interpreting the y-intercept as the approximate average flux between the stream channel and the subsurface. This approach was applied for the two scenarios in the tilted V catchment for days 24 – 305 (after the initial period of instability), as shown in Figure 7. For this time period, the best-fit line had an R^2 value of >0.9999 for both losing and gaining streams. In the losing-stream scenario, average channel loss was approximated as 64.1 m^3/hr; average baseflow in the gaining-stream scenario was estimated as 16.9 m^3/hr (Figure 8). For comparison, the average and peak inflows were 19,600 m^3/hr and 161,000 m^3/hr, respectively. The difference in order of magnitude between the inflow and the estimated subsurface exchanges can be attributed to the short reach length over which exchanges could occur.

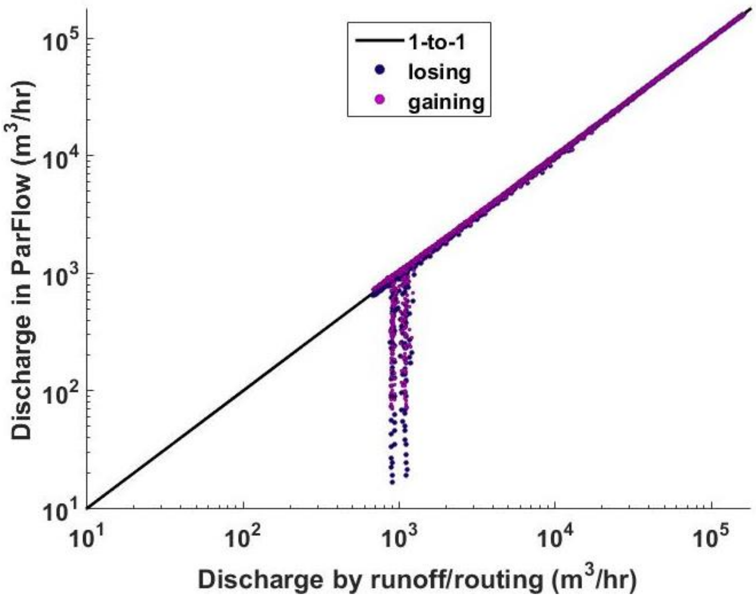

Figure 7. Outlet discharge in tilted V catchment: routing/runoff prediction versus model

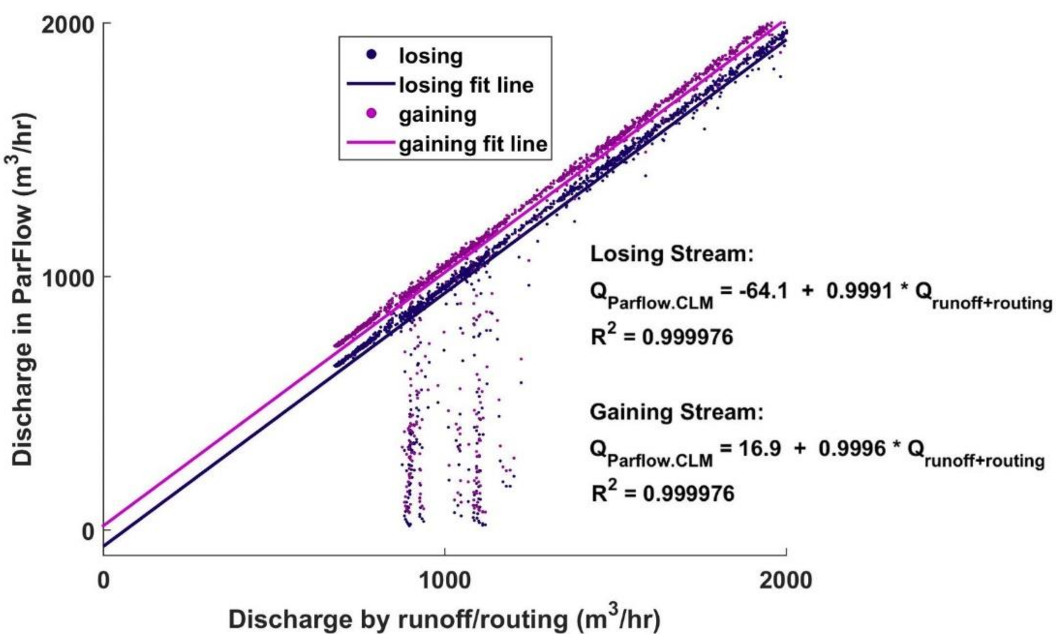

Figure 8. Outlet discharge in tilted V catchment: routing/runoff prediction versus model and fit lines (y-intercepts represent exchange with subsurface)

Thompson Creek Simulation

Spin-up

Following the successful test of the inlet flow method in the synthetic domain, the same process was repeated for the Thompson Creek catchment. The simulation period was selected such that the upstream flow was in baseflow (low flow) conditions at the beginning and end: October 5, 2015 – February 5, 2016. During spin-up, injection of upstream flow propagated to the outlet (22 km downstream) within one day. After this point, the magnitude of outflow was similar to inflow, and remaining changes could be attributed to the varying groundwater contribution as the subsurface conditions equilibrated.

Due to time constraints, a rigorous spin-up was not completed in the Thompson Creek domain. The 123-day simulation was run after two spin-up years (one initial run and one recursive run), which followed 130 days of steady-state spin-up (phases I and II). The model was run for an arbitrary period of 120 days with ParFlow only, then an additional 10 days with constant rainfall in CLM, before completing the two spin-up years. Table 5 describes the state of spin-up metrics at the end of each phase. In fact, percent changes in state variables were very small by the end of phase II. However, additional recursive runs of the spin-up year should have been completed to meet the criteria used in the tilted V domain. A total of 3607 CPU-hours were required for the completed level of spin-up.

Table 5. Stop criteria at the end of each phase of spin-up for Thompson Creek catchment

	Spin-up stop times (model days)	S_{GW}	S_{unsat}	Q_{outlet}	$\overline{DTW}$
Phase I (steady-state, ParFlow only)	Percent change after 120 days	-0.005%	0.002%	-1.095%	+0.001%
	Slope of %-change after 120 days (% per hr)	<0.001	-0.002	-0.007	-(<0.001)
Phase II steady-state with CLM)	Percent change after 10 days	-0.001%	-0.001%	-0.089%	<0.001%
	Slope of %-change after 10 days (% per hr)	0.002	-0.005	-0.025	- (<0.001)
Phase III (recursive 1-year runs)	Percent change in end-of-year storage from first spin-up year to second	4.96%	-10.80%	-2.68%	-1.44%

Simulation

The transient simulation for the Thompson Creek catchment was completed twice – once using CLM output from the end of the recursive run as the CLM initial condition, the second time using simple pre-defined conditions. Interestingly, the simple initial conditions performed better early in the simulation, but using recursive CLM conditions produced a better hydrograph later on (Figure 9).

Modeled discharge was lower than measured discharge for most of the simulation period in both model runs; this may be due to exaggerated groundwater interactions caused by the simplified subsurface domain and the inadequate model spin-up. For more accurate matching to the measured outflow hydrograph, the implementation and calibration of appropriate heterogeneous subsurface properties would be recommended. Because the initial state of CLM variables was the only difference in the two simulations, the differences in model behavior were attributed to land surface processes and problems in the coupling between ParFlow and CLM. For days 54 – 123, Run 1 performed very well, with a Nash-Sutcliffe model efficiency of 0.945 (Nash and Sutcliffe 1970). This is similar to the behavior seen in the tilted V domain (Figure 6), in which modeled discharge exhibited discontinuous extreme values early in the simulation, then began matching predicted outflow. Run 2, on the other hand, suddenly failed to perform after 91 days. This implies that using the CLM state at the end of spin-up is indeed the better option, but unknown problems are occurring early on, in spite of long spin-up periods.

Figure 10 illustrates groundwater elevation contours at different times during a flood. The simulations in the Thompson Creek domain demonstrate the applicability of ParFlow.CLM with an upstream flow boundary to study groundwater response to flood pulses from upstream.

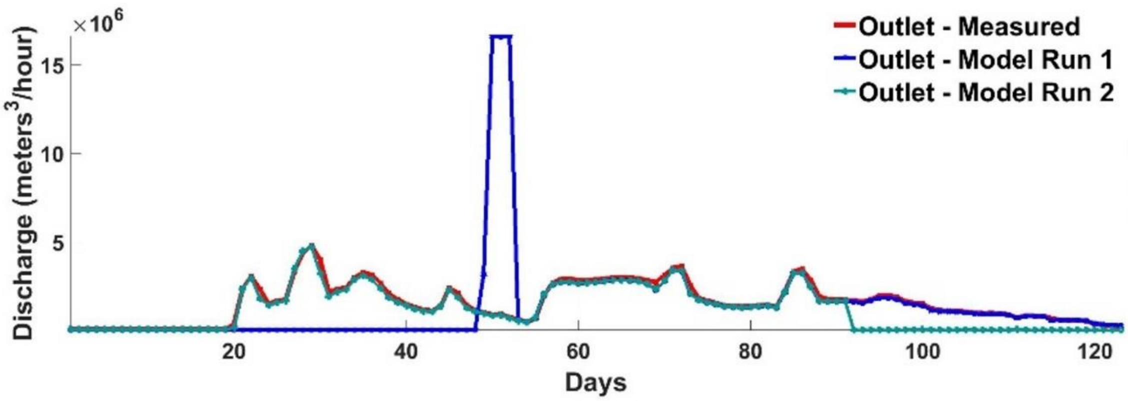

Figure 9. Hydrographs for Thompson Creek catchment

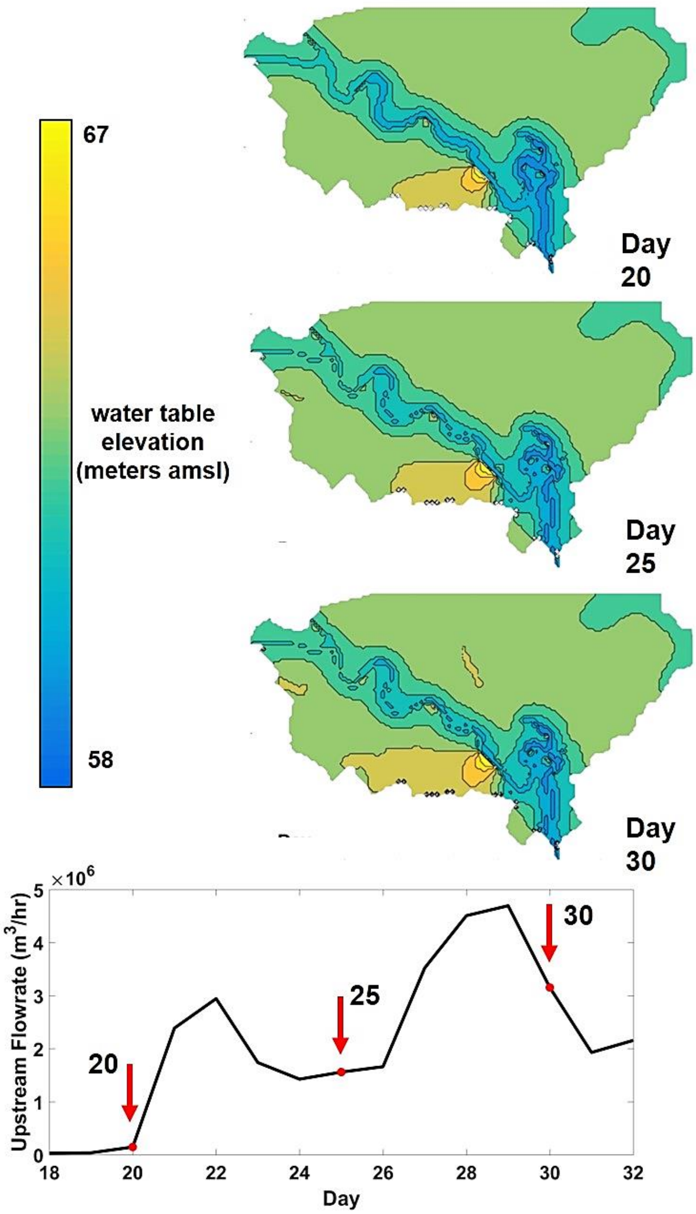

Figure 10. Groundwater table elevation at different points on a flood hydrograph

Water Balance

For each timestep of Run 1, errors in the water balance closure were within 0.2% of the total water storage volume, and 94% of errors were within 0.01% of total storage. Closure error at each timestep ($error_{WB}$) was defined as the difference between net inflow to the domain and change in the total domain storage:

$$error_{WB} = (\Sigma Q_{in} - \Sigma Q_{out}) - (V_{end-of-period} - V_{start-of-period}) \quad \text{Equation 14}$$

where V is the total volume of water stored in the domain, including surface, unsaturated, and saturated storage. The net inflow term in Equation 14 is defined as:

$$\Sigma Q_{in} - \Sigma Q_{out} = (Q_{inlet} + A_w * P) - (\mathrm{A_w} * \overline{q_{ET}} + Q_{outlet} + Q_{BC,out}) \quad \text{Equation 15}$$

in which $Q_{BC,out}$ represents net volumetric flux in the subsurface out of any boundaries. Water balance terms were only calculated for days 54 – 123. Fluxes and domain storage over time are shown in Figure 11. Overall, streamflow at the upstream boundary accounted for over 99.5% of average inflow to the domain (the rest being rainfall). Discharge at the outlet made up >99.9% of outflows; evapotranspiration accounted for the remainder, as all subsurface boundaries in this domain were zero-flow boundaries. However, total net inflow for days 54 – 123 was 3.0×10^7 m^3, and total change in storage was -9.3×10^5 m^3. Complete meteorological forcing data was not available for the simulation period. Because an accurate representation of land surface processes was not the goal for this simulation, simple estimates were used for radiation and wind data. Shortwave radiation values are estimated based on hour-of-day averages from the tilted

V simulation period. Longwave radiation and wind speed were set to zero, so evapotranspiration is not represented accurately. Other errors are most likely attributable to round-off errors in ParFlow outputs.

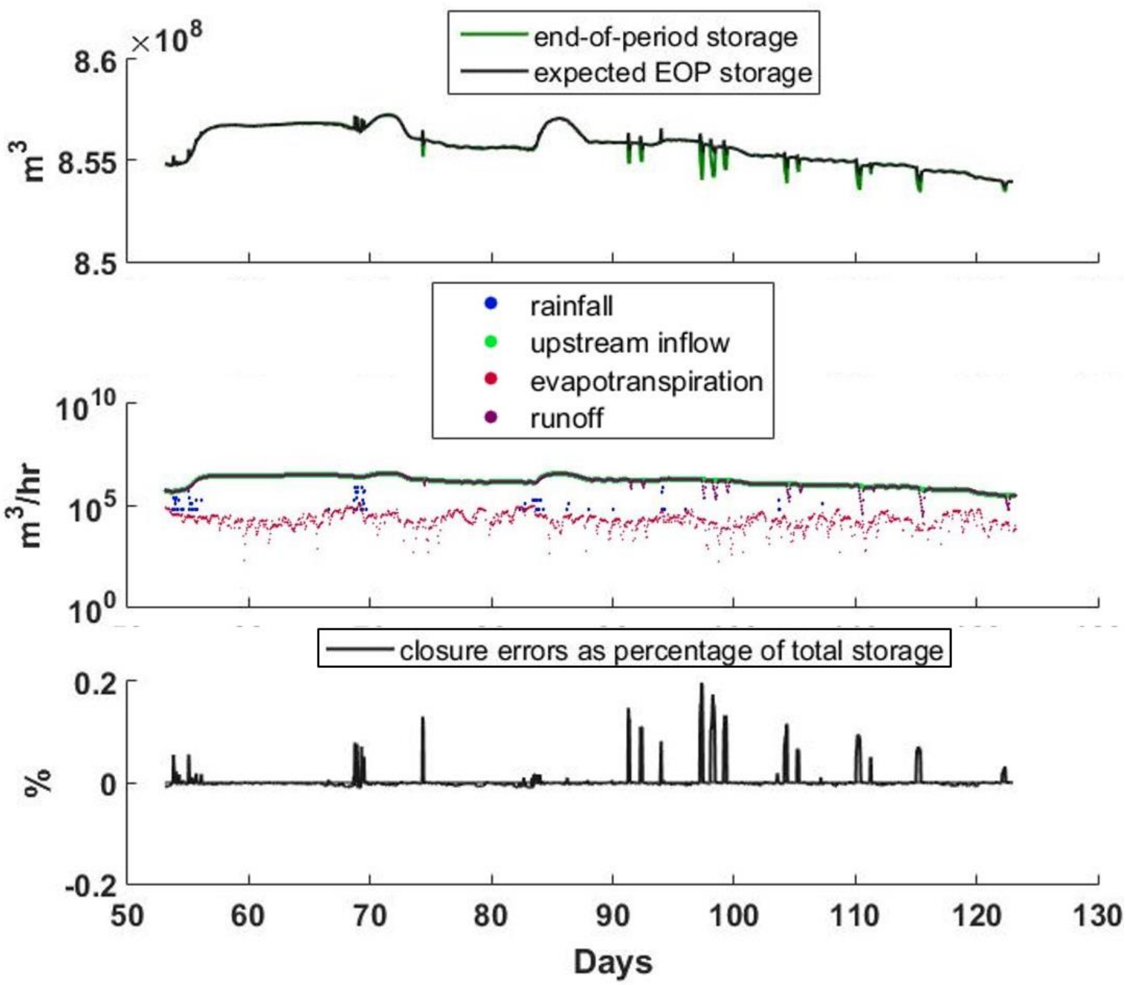

Figure 11. Total domain storage (top), inflows and outflows over time (middle), and water balance closure errors (bottom)

Summary

ParFlow.CLM is a powerful tool for modeling integrated hydrologic processes in large, complex domains. A critical weakness of ParFlow is its inability to incorporate time-series of streamflow as an upstream boundary condition, and previous studies have been limited to headwater catchments. A method for introducing transient inflow at an upstream boundary has been demonstrated in an idealized domain and a more realistic catchment. The method is easily repeatable, requiring only a little additional pre-processing of input forcing data and the addition of injection-induced streamflow during model spin-up. Injection of steady-state flow is a reliable method for initializing streamflow, which quickly propagated downstream, relative to the time required for initializing subsurface conditions.

The modeled discharge in the tilted V domain was compared to predicted discharge using a combination of traditional rainfall-runoff calculations and hydraulic routing. The best-fit offset between predicted and modeled discharge represented the interactions with the subsurface afforded by a coupled model. Although runoff is small in a small domain and routing is almost unnecessary for such a short reach (250 m), this comparison method could be applied for longer reaches or more complex stream systems to demonstrate the impact of a coupled model over an uncoupled surface flow model which performs such routing calculations.

When compared with measured outlet discharge in a simplified case for the Thompson Creek catchment, it is apparent that the initial state of CLM variables greatly affects model performance. Most importantly, the method developed here for incorporating transient streamflow at an upstream boundary can be used to study subsurface responses to surface conditions, such as flood pulses from upstream.

CHAPTER III

A CONCEPTUAL EARTH SYSTEMS MODEL FOR THE BRAZOS RIVER ALLUVIUM AQUIFER

Introduction

Traditionally, groundwater is modeled in a fully-saturated framework. However, for many shallow aquifers, and particularly those in connection with a river, a saturated-flow model is insufficient. In Texas, Oklahoma, Kansas, and the Mississippi River Valley, alluvial floodplain aquifers are found in river valleys. Additionally, all of these areas are important for agriculture, which is dependent on soil moisture conditions. In such systems, it is important to assess the hydrologic cycle holistically, rather than dividing the groundwater, soil, and surface water components.

Here, I present a conceptual model for representing the Brazos River, the Brazos River Alluvium Aquifer, and overlying vegetation in a fully-integrated Earth systems model. This model is intended for long-term use by researchers in the Texas Water Observatory network to answer questions related to physical processes and water resource management.

Texas Water Observatory

In 2015, the Texas A&M Research Development Fund and three Texas A&M colleges supported the initiation of the Texas Water Observatory, or "TWO." The TWO project is intended to be a multi-scale hydrologic monitoring network, which also includes the application of observed data for improved understanding and management of water resources in Texas and similar environments. The primary objectives of TWO are to (1) collect hydrology-related field data, (2) model integrated physical processes, (3) analyze and assess observed and modeled data for decision-making applications, and (4) disseminate real-time and value-added data through a web-based data portal.

Brazos River Alluvium Aquifer

The Texas Water Observatory is building its initial network within the southeastern Brazos River Corridor. In this region, the Brazos River is underlain by the Brazos River Alluvium Aquifer (BRAA), a groundwater reservoir in the river's floodplain. Understanding the interactions of this aquifer with the river and land systems is a fundamental part of the TWO objectives. The BRAA is in direct hydraulic connection with the river for 610 km, making it an important component of the river basin's hydrologic system. Designated as a "minor aquifer" by the Texas Water Development Board (TWDB), the BRAA is used primarily for localized irrigation pumping. However, as projected water demand in Texas continues to grow, interest has been shown in developing the BRAA as a supplement to surface water supplies (O'Rourke 2006), and an increase in pumping for mining and irrigation was included in the 2016 Brazos G Regional Water Plan (TWDB 2015).

To more accurately inform regional and state water plans, the TWDB has developed a Groundwater Availability Model (GAM) of the BRAA using MODFLOW (Ewing and Jigmond 2016). However, as an alluvial floodplain aquifer in direct hydraulic connection with a river, this aquifer is more dependent than most upon surface and vadose zone processes. The capacity of MODFLOW to represent surface-subsurface interactions is limited, and data for estimating those processes is lacking as well.

Integrated Hydrologic Models for Real, Heterogeneous Domains

In a previous model, the BRAA was represented as a simplified, non-coupled, subsurface model that considered parallel, homogeneous layers discharging to a stream (Chakka and Munster 1996). Several researchers have discussed the importance of heterogeneity in the shallow subsurface. For example, saturated vertical connections through highly-permeable facies can create localized flow paths (Fleckenstein et al. 2006; Frei et al. 2009); gaining reaches may be losing in small patches or within certain layers of the hyporheic zone (Woessner 2000); and colmation may occur in a patchy fashion rather than clogging an entire reach of streambed (Treese et al. 2009). Even when a degree of spatial variability is accounted for, a modeled system may behave quite differently under different realizations of the heterogeneity structure, as demonstrated by Frei et al. (2009) and Fleckenstein et al. (2006). Their outputs revealed that in spite of similar model fit and mass balance between simulations, different realizations of subsurface variability alter the timing, spatial distribution, and net volumes of exchange across the stream-aquifer interface.

Several coupled models are now available, some of which have shown promise in dealing with heterogeneity. However, more studies are necessary to assess the skill of different modeling systems in facing these challenges. Sebben et al. (2013) have pointed out that the test cases most commonly used for evaluating and comparing integrated hydrologic models are based on homogeneous media and simplified forcing data.

Additional model evaluations will need in-depth, long-term field studies in real catchments. Such studies could potentially capture the strengths and weaknesses of different models for modeling heterogeneous systems. Additionally, surface-subsurface integrated models will best represent physical systems when they also incorporate land surface processes and atmospheric exchanges (Refsgaard et al. 1998; Shi et al. 2013).

A High-Order Watershed Model in ParFlow.CLM

The BRAA numerical model is the first of its kind in ParFlow.CLM – a large, heterogeneous, higher-order catchment. Because the watersheds included in the model domain are far downstream of the Brazos River headwaters, it will be an excellent large-scale test of the transient stream inflow method developed in the previous chapter. In fact, incorporating the high-temporal-resolution inflow method is a necessity for the numerical model, which is intended for a seven-year simulation using hourly forcing data. The model also incorporates a free drainage condition, whereas many previous ParFlow studies have used no-flow boundaries for all of the subsurface. Being developed within the Texas Water Observatory, this model will be able to take advantage of large data streams, which can be used to continually improve the model through calibration and later to validate the model. The calibrated model will then be a useful tool in understanding the hydrologic processes in the Brazos River Basin and Brazos River Alluvium Aquifer.

Study Area Description

The Brazos River Alluvium Aquifer (BRAA) is the only alluvial aquifer in Texas in direct hydraulic connection with a river for a significant distance. The BRAA has a footprint of approximately 2,850 km^2; it extends from Bosque County in the northwest to Fort Bend County in the southeast. The aquifer is restricted to floodplain sediments and is laterally bounded by older terrace alluvium.

Field Studies and Data Review

Geology

In 1967, Cronin and Wilson completed the first detailed characterization of the BRAA, assessing its geological and hydrogeological properties, as well as surface physiography, climate, and development in the region. The authors determined the alluvium structure to be upward fining from gravel of varying size to fine sand and occasional clay caps (Cronin and Wilson 1967). In particular, they noted that the bedrock contact at the base of the aquifer is generally easy to distinguish north of Hempstead, TX, making the basal surface more definite for modeling purposes.

Hydraulic Characteristics

Throughout the extent of the aquifer, water generally flows toward the river, and only a small component of subsurface flow is parallel to river flow (Cronin and Wilson 1967; Wrobleski 1996). However, flow configurations can vary; some reaches of the river were identified as losing reaches in a study of 2006 hydrographs (Ewing et al. 2016; Turco et al. 2007). Estimates for storage-related parameters have varied. The specific yield in the BRAA was estimated by Cronin and Wilson (1967) at a conservative value of 15%, which has been used in later studies of the alluvium aquifer (Ewing et al. 2016; O'Rourke 2006). Chakka and Munster (1997) assumed a homogeneous specific storage value of 1×10^{-6}. Wrobleski (1996) calculated specific yield values as low as 7.3×10^{-4} and storativity ranging from 1.5×10^{-4} to 1.1×10^{-3} from a pump test conducted near FM 60. The TWDB has modeled the BRAA with a storativity of 0.01, and they report that "all storage parameters were very insensitive (Ewing and Jigmond 2016, 2-30)." The USGS reviewed various data sources and reported transmissivities in the BRAA ranging from 27 to 2600 m^2/day (Shah and Houston 2007). Thick clay deposits, which overlie 63% of the aquifer within the study area, at depths of up to 18 m, produce localized confining conditions in the BRAA (Cronin and Wilson 1967), and Wrobleski (1996) suggests that semi-confined flow may even be induced by the fine sands in the upper aquifer strata.

Water Quality and Use

In general the groundwater in the BRAA is too high in dissolved solids for domestic use, but it is frequently used for irrigation, although there is a risk of salinity hazard (Ewing et al. 2016). Total dissolved solids concentrations in the groundwater within the proposed model area vary from <500 to >1,000 milligrams per liter (Chowdhury et al. 2010). Nitrate also poses a concern to any domestic use; three of eleven measurements were above the 10 mg/L maximum contaminant level (MCL) between 2003 and 2013. Additionally, iron, manganese, sulfate, and chloride were found to be above the MCL in five, six, two, and one out of eleven tests, respectively (TCEQ 2014b).

Several streams in the study area are listed by the TCEQ as impaired, including Davidson Creek, Thompson Creek and its tributaries, and most of the channels in the Navasota River basin, including the river itself (Figure 12). The creeks in the Brazos River Basin are all Category 5 impaired, mostly by bacterial presence, with a few instances of depressed dissolved oxygen. Additionally, Somerville Lake, from which flows Yegua Creek, is listed as impaired for pH levels (TCEQ 2014a).

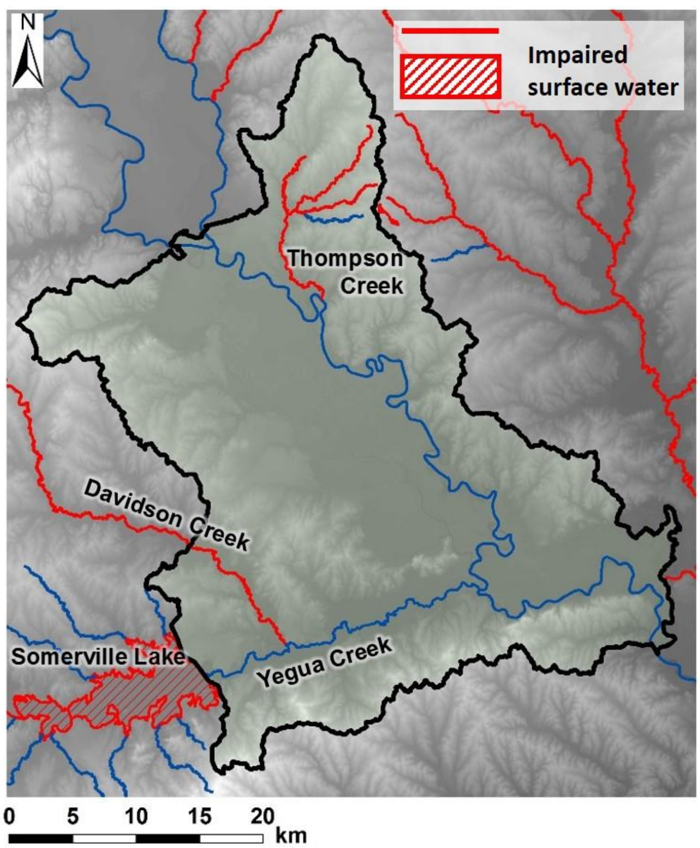

Figure 12. Impaired waterways and reservoir near Brazos and Burleson Counties, TX

Previous Modeling Studies

River Stage and Aquifer Response (field-scale, VS2DT)

In 1996, Chakka and Munster studied the relationship between river stage and the river-aquifer exchange flux in the BRAA using the USGS modeling system “Variably Saturated Two-Dimensional Transport” (VS2DT). Their model focused on processes in and near the hyporheic zone and so was limited to a field-scale extent: 403 m in the direction of flow (toward the river), and 12.7 m vertically. The system was represented as two constant-thickness, homogeneous layers (clay and coarse alluvium) discharging to a stream with time-varying head. Although VS2DT models variably-saturated conditions (both vadose and saturated zone), it is not coupled with a surface flow model. The river stage was represented as a specified-head boundary in the 2-D model, which varied daily based on field measurements. This model confirmed that the aquifer discharges as baseflow when the river stage is low, but receives recharge from the river when stage is higher. However, this conclusion is limited to the field where the data were obtained; Turco et al. (2007) demonstrated the variability of gain/loss conditions and Rhodes (2016) reported that the groundwater response to flood stage was often limited to near-river bank storage.

TWDB Groundwater Availability Model (aquifer-scale, MODFLOW)

The conceptual model of the TWDB GAM for the BRAA (Ewing et al. 2016) includes a thorough review of prior studies in the aquifer and an outline of methods used in the GAM formulation. The BRAA GAM incorporates data from the models for underlying aquifers (Carrizo-Wilcox, Gulf Coast, Queen City, Sparta, and Yegua-Jackson) to account for exchange between the BRAA and shallow subsystems of those aquifers.

The numerical GAM, completed in MODFLOW, incorporates several MODFLOW packages to address surface interactions: Recharge, Evapotranspiration, River, Drain, and Streamflow-Routing packages (Ewing and Jigmond 2016). However, it remains an uncoupled model and must rely on available data to estimate surface-subsurface interactions. For example, the GAM reports that available baseflow measurements were not adequate as “quantitative targets for transient calibrations;” short-term hydrograph separation analyses were only used to assess whether reaches should have been losing or gaining (Ewing and Jigmond 2016, 3-2). In addition, the base surface of the aquifer in the TWDB model was developed based on the assumption that the top of the aquifer is the land surface (Ewing et al. 2016). Considering that much of the BRAA is overlain by clay caps as thick as 18 m, such a formulation may misrepresent the available storage volume.

Study Domain

The domain for this model is the region between SH-21 and the Brazos-Navasota confluence near SH-105 in Brazos, Burleson, and Washington counties (Figure 13). The portion of the aquifer within the model domain is approximately 17% of the entire BRAA areal extent. Although the model does not include the full aquifer extent, the study section is a valuable region for irrigation withdrawals and has sufficient data available to assess numerical model performance. This study area was selected based on the availability of spatial and temporal data, the inclusion of Texas A&M University Brazos River Hydrogeologic Field Site, and the locations of stream gages with consistent historical data availability (Figure 14). The field site is an experimental data collection site that has included nine monitoring well nests, a river well, a water table well, a weather station, and a nearby stream gage at different periods since 1995 (Munster et al. 1996).

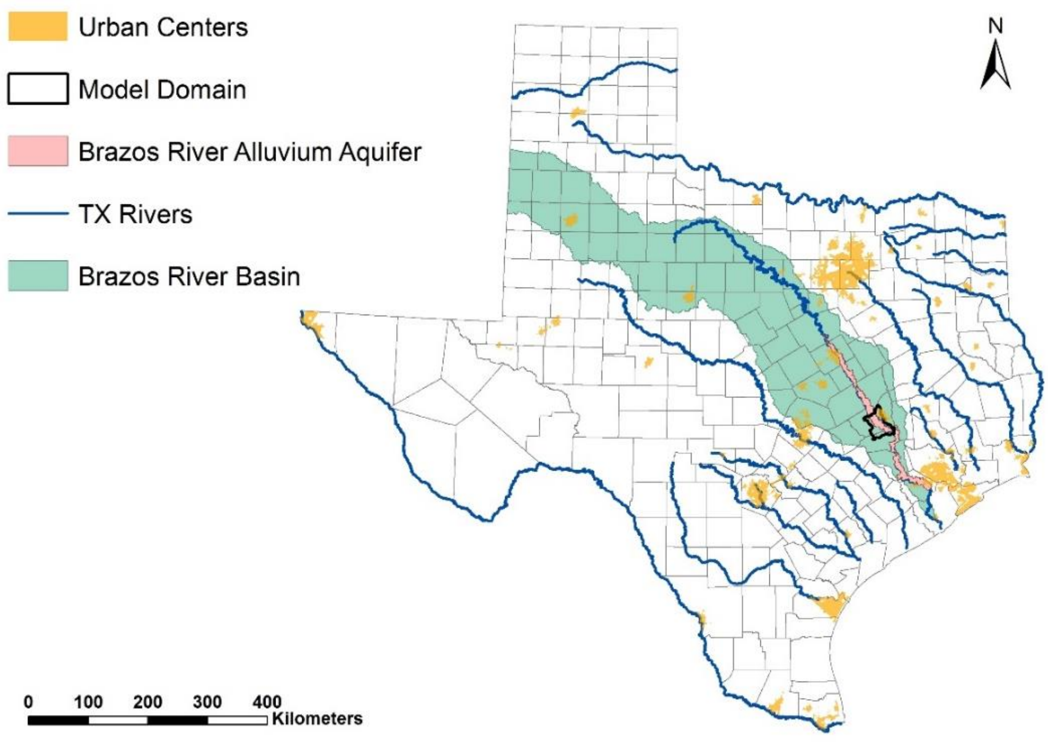

Figure 13. Brazos River Alluvium Aquifer study area location

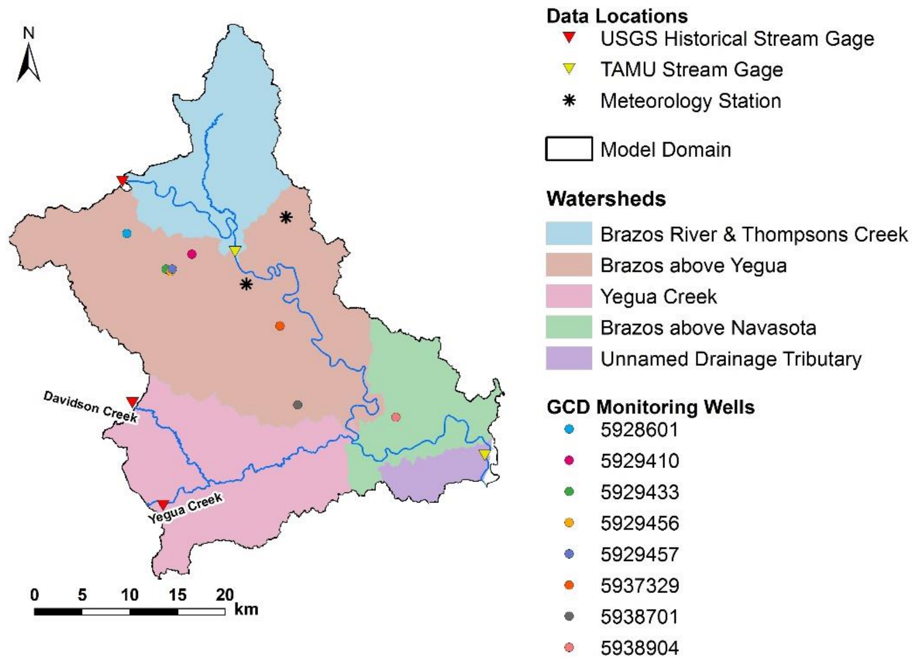

Figure 14. Watersheds and data measurement locations

Long-term streamflow data are available on the Brazos River at SH-21 and SH-105, making these good upstream and downstream boundary points for the model. The extent was then constrained by topography so that the lateral bounds of the model follow watershed divides (Figure 14). Land use in the study area is primarily agricultural (Figure 15). Developed urban areas and woodland vegetation are also prevalent, but are mostly limited to the upland terraces. Vertisols dominate the surficial soils in the alluvial floodplain and along the Yegua Creek; these soils are characterized by high clay content and shrink-swell behavior that produces cracking (USDA-NRCS 1999). The terraces are primarily covered by alfisols (Figure 16).

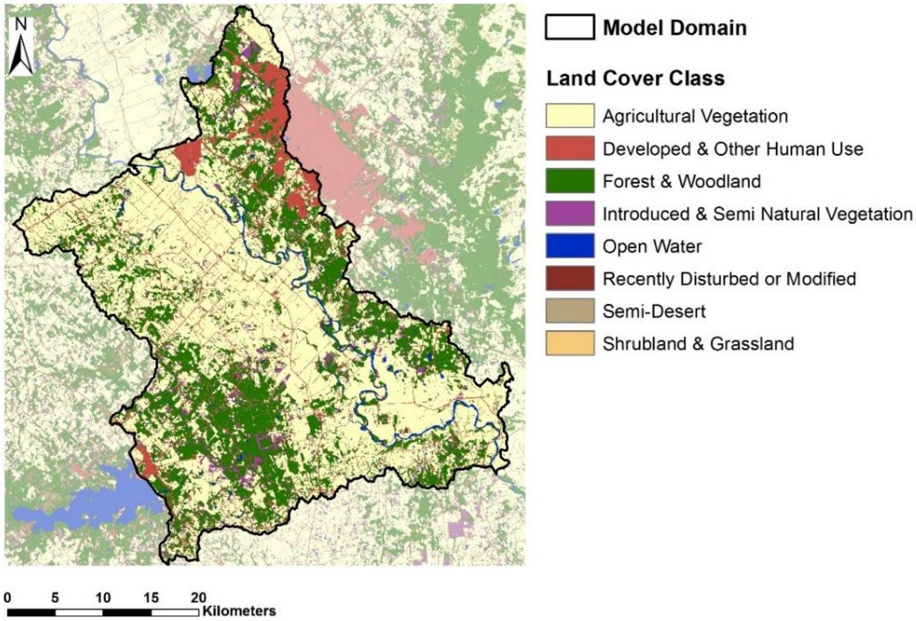

Figure 15. Land cover

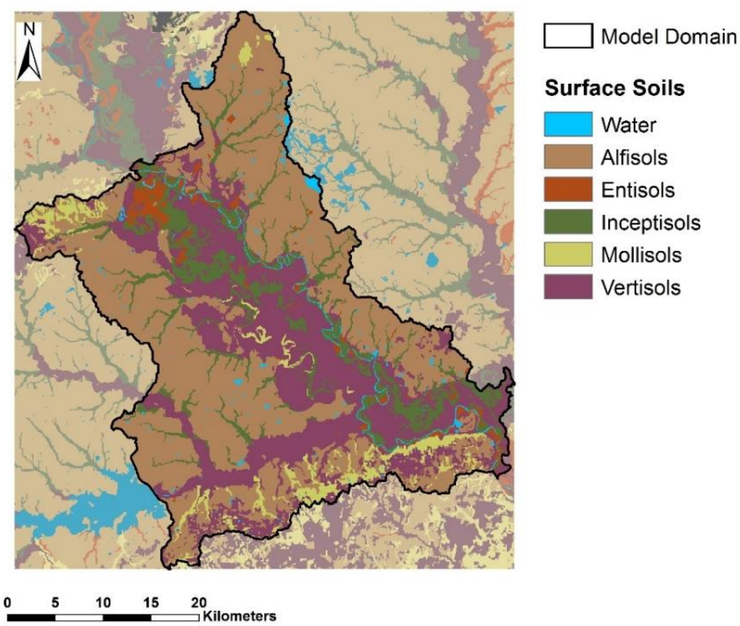

Figure 16. Surface soil by taxonomic order

Underlying Formations

Within the selected model domain, 16% of the BRAA is underlain by the Gulf Coast Aquifer, and 71% is underlain by the Yegua-Jackson aquifer. However, Knox et al. (2007) suggest that the Yegua-Jackson outcrop is “interrupted” by the Brazos River floodplain alluvium. Rather than a direct contact with the underlying aquifer, low-permeability shale forms the bedrock beneath much of the alluvium aquifer in this area. Although some vertical flow between these aquifers and the alluvium is possible, the quantity is most likely very small (Chowdhury et al. 2010). This leakage will not be considered in the present conceptual model.

Streams

The Brazos River meanders across its flood plain as it flows southeast toward the Gulf of Mexico. The model domain includes 95 km of the Brazos River. The flood plain is also crossed by several small streams, some of which meander alongside the Brazos River for several kilometers before joining it. East of the model area, the Navasota river flows southward until its confluence with the Brazos, just south of SH-105. Upstream from this confluence, the Yegua Creek also joins the Brazos River after leaving Somerville Lake. Stream discharge data are available for Yegua Creek at its outflow from the lake and for the Brazos River at SH-21 and SH-105 (USGS 2016c). However, no continuous discharge data are available for the Navasota River near the study area. Because of this, river stage in the Navasota will be approximated based on the difference in elevation of points on the river and at the Brazos River stream gage at SH 105, as shown in the USGS National Elevation Dataset (USGS 2016a).

Climate and Hydrology

Average annual precipitation in the study area is 1020 mm, but extreme drought conditions and intense flooding have occurred in the past decade. The worst one-year drought on record occurred in 2011, and spring floods have greatly exceeded normal conditions (Figure 17). As a result, the Brazos River has experienced highly variable stage with large flood pulses (Figure 18). As the alluvial aquifer becomes more important as a water source, it will be helpful to determine how the aquifer responds in these extreme cases.

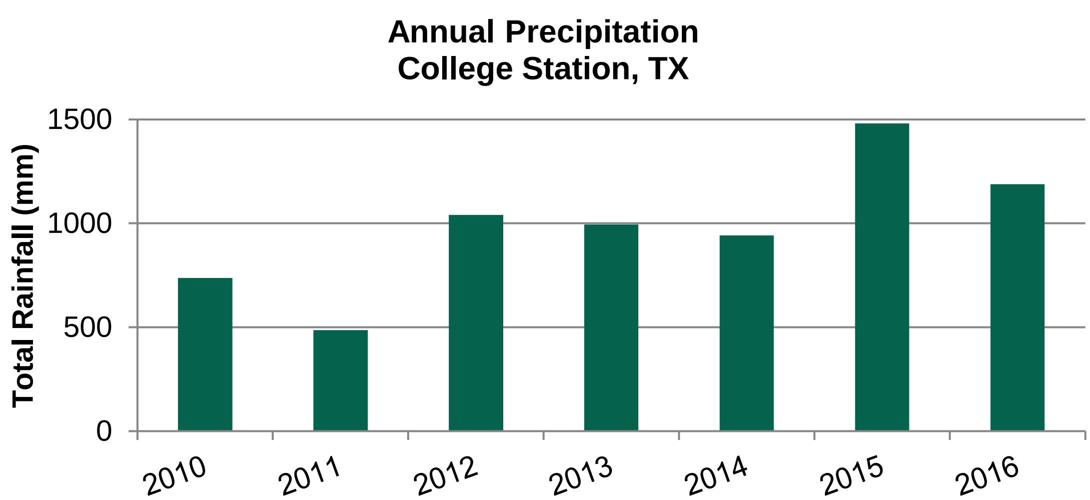

Figure 17. Annual rainfall totals in study area

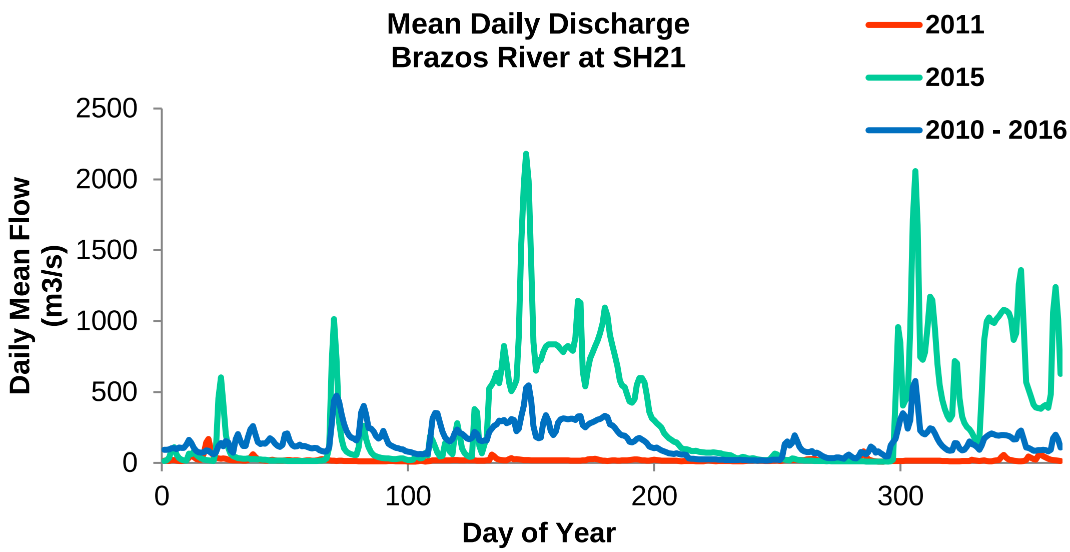

Figure 18. Streamflow at upstream boundary of study area

Model Formulation

Extent and Discretization

The computational domain is 581 by 522 cells horizontally (north-south and west-east, respectively), and includes 152 vertical layers. However, the active model domain is an irregular shape defined by the topographic watershed divides and the spatially-variable thickness of the aquifer and terraces. Because of the formulation of the active domain shape, only 1,774,902 of the 46,098,864 cells in the 3-dimensional grid are active (3.9%). ParFlow has unstructured grid capabilities only in the vertical direction; the BRAA model uses a uniform, structured grid. Each cell is 100 m x 100 m horizontally and 1 m deep. Because of the large number of inactive cells, the

PFMGOctree preconditioner will be used in the numerical model, as recommended by the ParFlow User's Manual (Maxwell et al. 2016).

Model Zones

The x-y domain of the model area has been divided into three zones – the west and east terraces, and the aquifer (Figure 19). Groundwater flow will only be solved within the extent of the alluvium aquifer, but the terraces are included to account for overland flow between watershed divides. Although only the top 2 m of soil are considered relevant for runoff partitioning, the terrace zones extend to a depth of 10 meters. The variation in topography, which for 100-m x 100-m grid cells can be greater than 2 meters in elevation, caused discontinuity in the model domain when only 2 meters of terrace soil were included. The model cells in the aquifer zone are active between the land surface and the base of the aquifer, which has been defined here as the horizon between alluvium materials and underlying shale.

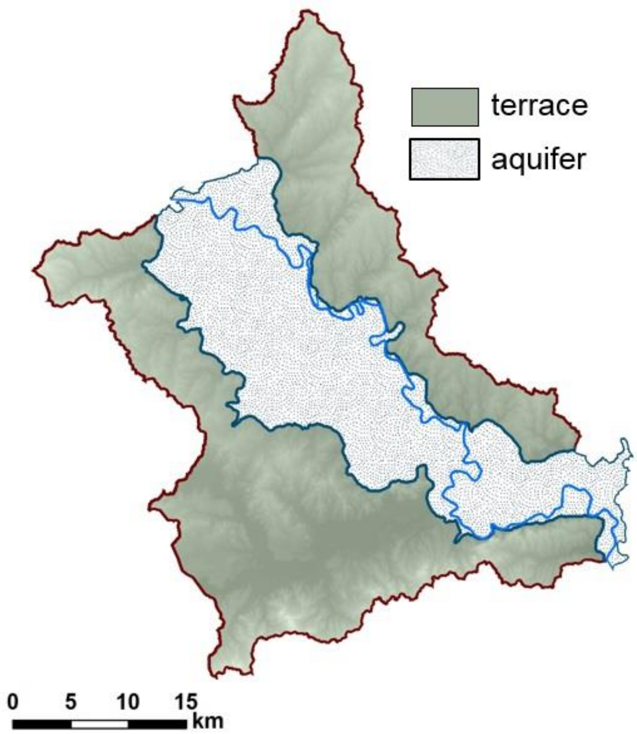

Figure 19. Terrace and aquifer zones of model domain

Boundary Conditions

Land Surface and Surface Inflow

The upper boundary of the model domain is the land surface; the pressure continuity condition provides a flux value at the surface, which varies in both time and space depending on the distribution of surface pressures. The coupled land-surface model CLM partitions precipitation between infiltration and runoff, then provides pressure inputs to the top surface of the ParFlow model. ParFlow then solves subsurface saturation and returns saturation data to CLM (Maxwell and Miller 2005). Additionally, the transient stream inflow method described in the previous chapter is used to introduce time-varying streamflow at the point where the Brazos River enters the domain. Figure 20 and Figure 21 illustrate the various processes and inputs in the model. Long-term streamflow data at SH-21 (USGS 2016c) will be used as the transient inflow boundary condition.

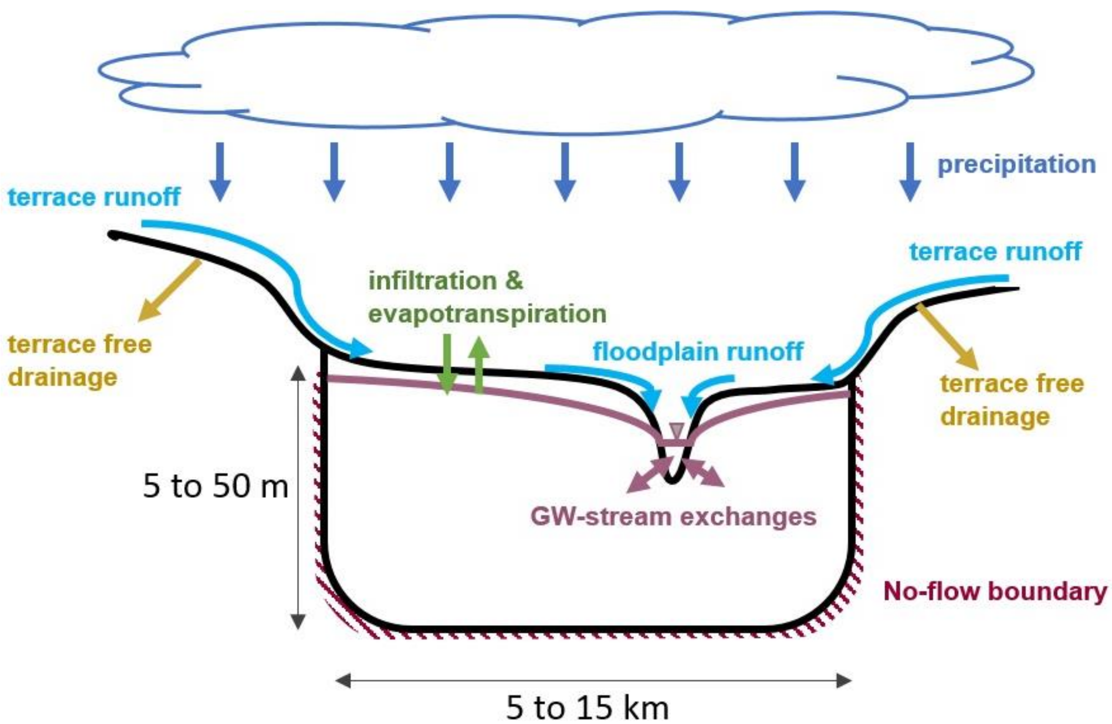

Figure 20. Conceptual model, cross-sectional view

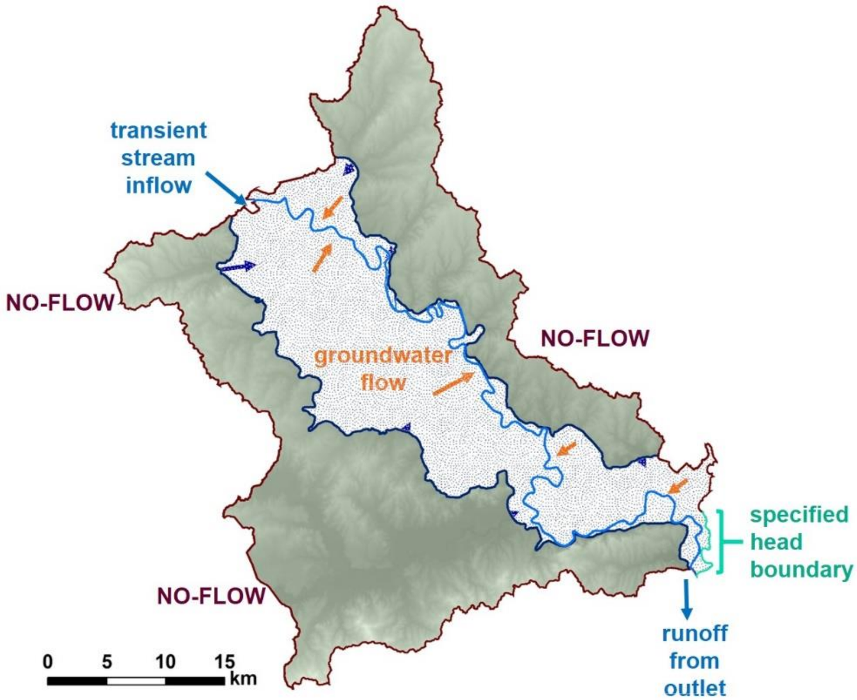

Figure 21. Conceptual model, plan view

Free Drainage Boundaries

For each terrace (east and west), a constant head (Dirichlet) boundary condition is applied to the bottom surface. Because the terraces are being used to simulate infiltration/runoff partitioning only, any infiltration can be allowed to drain out of the model domain. This infiltration eventually becomes recharge to the underlying Yegua-Jackson and Gulf Coast aquifers, which are not included in this model. ParFlow does not have a built-in free drainage condition, so this is accomplished by setting the water table to a constant elevation 1 meter below the base of the terrace zones.

Navasota River as a Head Boundary

The second Dirichlet condition is applied on the southeast edge of the domain, which is formed by an 8.5-km reach of the Navasota River, just upstream of its confluence with the Brazos River. Here, the Navasota is at a lower elevation than the Brazos, and the distance between is small enough that groundwater flows directly from the Brazos to the Navasota. A specified-head boundary condition will be applied such that for each point along the reach, hydraulic head is defined as:

$$H_{BC}(x_{BC}, t) = H_{gage}(t) + H_{Navasota}(x_{BC}, t_0) - H_{gage}(t_0) \qquad \text{Equation 16}$$

where $H_{BC}(x, t)$ is the specified head on the boundary, x_{BC} is distance from the gage at SH-105, t is time, $H_{gage}(t)$ is the measured water surface elevation of the Brazos River at SH-105, $H_{Navasota}(x_{BC}, t_0)$ is the elevation of the Navasota River on digital elevation map (DEM considered to be taken at $t = t_0$), and $H_{gage}(t_0)$ is the elevation at stream gage location on digital elevation map. Because of the restrictions on transient boundary conditions, the $H_{gage}(t)$ and $H_{BC}(x, t)$ terms must be defined as piecewise functions, such that head is constant for certain periods, rather than defined at each timestep (Equation 17).The ParFlow "cycle" for this boundary lasts the entire simulation period and is divided into sub-periods based on threshold levels of river stage in the Navasota, between which the assigned head for that sub-period (i) is the average head over the period (Equation 18).

$$H_{gage}(t) = \{H_i, \qquad t_{i-1} < t < t_i \qquad \text{Equation 17}$$

$$H_i = \int_{t_{i-1}}^{t_i} H(t)dt, \text{ where } t_i = t \; at \; which \; H(t) > H_i \qquad \text{Equation 18}$$

No-Flow Boundaries

The remainder of the domain is bounded by a zero-flux Neumann condition. This assumes that no groundwater flows horizontally in and out of the domain except via baseflow to the Brazos and Navasota Rivers and that there is no vertical exchange with underlying formations. Previous studies have suggested that such vertical exchanges are in fact very small (Chowdhury et al. 2010). At the northern edge of the domain, the model boundary follows a topographic flow line based on the assumption that groundwater flow mimics surface water flow here, such that the component of groundwater flow parallel to the river can be approximated as negligible.

Anisotropy for a Pseudo-Boundary Condition

At the subsurface interface of the shallow terrace zones and the deeper alluvium aquifer, an internal pseudo-boundary was created to prevent water in the aquifer from exiting through the terrace free drainage boundary. A "wall" was generated in the terrace cells adjacent to the aquifer, from surface to the base (10 meters total). The "wall" cells were assigned a horizontal-to-vertical anisotropy ratio of 0.01, which permits vertical normal drainage, but greatly reduces horizontal flow from the aquifer into and through the terrace material. The remainder of the domain, in both terraces and the aquifer, is considered to be isotropic.

Hydraulic Parameters

Surficial Soils

The top 2 meters in the model are designated as surface soil units, and properties are defined based on soil map units from soil surveys (USDA-NRCS 2016). The remaining depth of the terrace zones will also be assigned surface soil properties for simplicity, as the terraces are only intended to generate appropriate infiltration/runoff partitioning of precipitation. Saturated hydraulic conductivity values for the soils were obtained from the soil survey data; K_{sat} in surface soils ranges from 7.7x10^{-5} to 3.3x10^{-1} m/hr. The van Genuchten model will be applied to represent variably saturated flow dynamics. Rosetta (Schaap et al., 2001) will be used to compile van Genuchten parameters for the surface soils.

Aquifer Geology

Within the BRAA zone, geological layers defined by borehole data will be included from 2 m below land surface down to the basal surface of the aquifer. The conceptual model for the geologic layers (Figure 22) was constructed using the software package Groundwater Modeling System (GMS, Aquaveo, 2016). Drilling log data for 75 boreholes, which included 12 material types in and above the alluvium aquifer layers, were re-classified into five material groups: shale, clay, gravel, sand, and sand/gravel mix. The horizon produced by the GMS interpolation between the coarser alluvium and the underlying shale is used to define the basal surface of the aquifer. Material groups are given porosity values based on a previous modeling study in VS2DT (Chakka and Munster 1997).

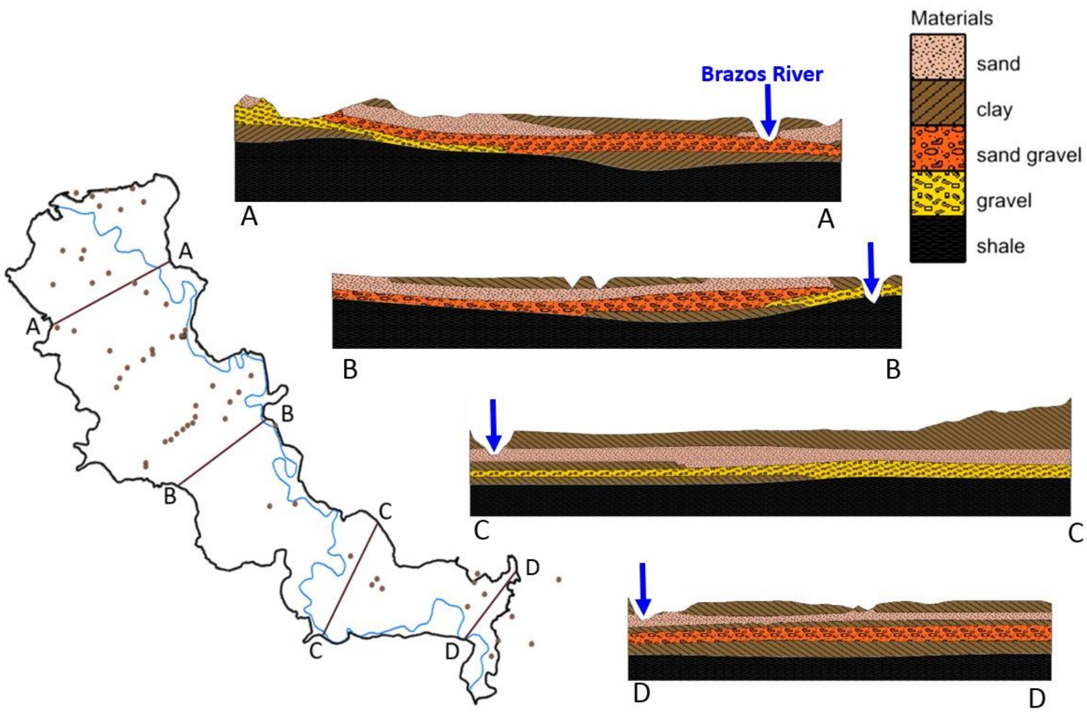

Figure 22. Cross-sections of GMS-generated geology model with locations of cross-sections and boreholes in study area of BRAA (vertical exaggeration = 35)

To account for the presence of macropores that form in the cracking clay, the clay was assigned the porosity value estimated for “silty clay” rather than “clay.” The properties of the shale layer are arbitrarily set very low, as this represents the no-flow base surface of the aquifer (Table 6). Because the water table is typically 5 to 10 m below the land surface in the study area, some of the non-surficial layers will be unsaturated, so van Genuchten properties will be applied here as well.

Hydraulic conductivity for each material class was estimated using transmissivity data available at 59 wells in the study area. Because borehole data were typically unavailable at wells with transmissivity estimates, boreholes were generated from the GMS geology model at those locations. Each material layer in the model was assigned an initial conductivity value (k_i); a modeled transmissivity was then calculated for each borehole (Equations 19 and 20). The k_i values were optimized using a simple trial & error algorithm implemented in MATLAB to minimize the root mean squared error ($RMSE$, Equation 21) between modeled and measured transmissivity.

$$K_{eff} = \frac{\Sigma(k_i * b_i)}{\Sigma b_i} \qquad \text{Equation 19}$$

$$T_{modeled} = K_{eff} * b \qquad \text{Equation 20}$$

$$RMSE = \sqrt{(\frac{1}{N} * \Sigma((T_{modeled} - T_{measured})^2))} \qquad \text{Equation 21}$$

Here, k_i and b_i refer to the assigned conductivity value and thickness of each layer, b is the total thickness of the aquifer materials in the model at that location, K_{eff} is an effective hydraulic conductivity for horizontal flow into the borehole across all layers in the aquifer, N is the number of boreholes, $T_{modeled}$ is the calculated transmissivity, and $T_{measured}$ is estimated from a pump test or specific capacity. All layers included in the optimization were assumed to be fully saturated. Table 6 lists the final conductivity values estimated from this method.

Table 6. Hydraulic properties for aquifer layers in BRAA model

Reclassified Material	Original Material	Saturated Hydraulic Conductivity (m/hr)	Porosity
Sand	sand sandy clay sandy shale	1.5	0.30
Sand/gravel mix	sand/gravel mix	1.2	0.30
Gravel	gravel	0.75	0.30
Clay	clay clay/gravel mix clay/gravel/sand mix	0.20 at surface 0.037 in lenses 0.43 near base	0.40
Shale	shale limestone clay/shale rock	1.0×10^{-6}	0.001

Validation Data

Once spin-up of the numerical model has been completed, it will be validated against historical stream discharge and water level data. The purpose of the model is to accurately represent both groundwater and surface water processes as they interact with each other. For example, aquifer levels measured at the A&M Hydrogeologic Field Site demonstrate that the aquifer responds quickly to drought and flood conditions (Figure 23). These measurements were taken only 430 meters away from the river, and it is a shallow aquifer, so the rapid response to river stage is reasonable. Modeled groundwater levels should be compared to data both at near-river monitoring wells and others in the floodplain (Figure 24). Stream discharge will be compared to gage data near SH-105, at the outlet of the study area.

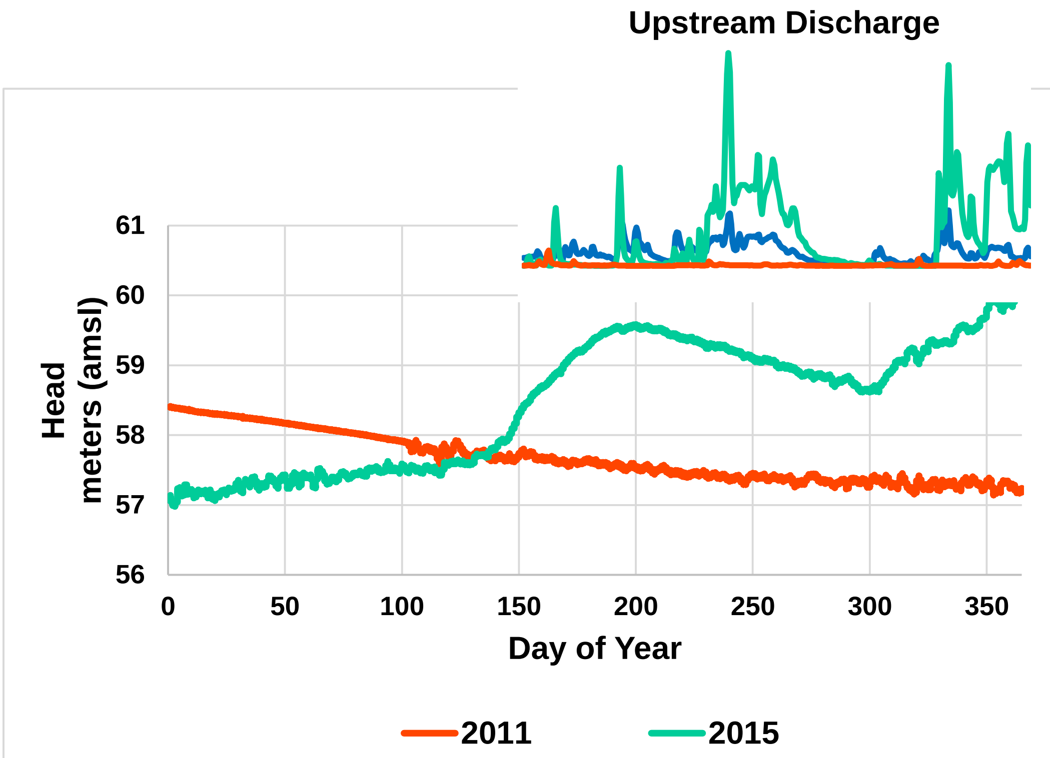

Figure 23. Measured head in a well 430 m from the river, 22 km below the upstream boundary

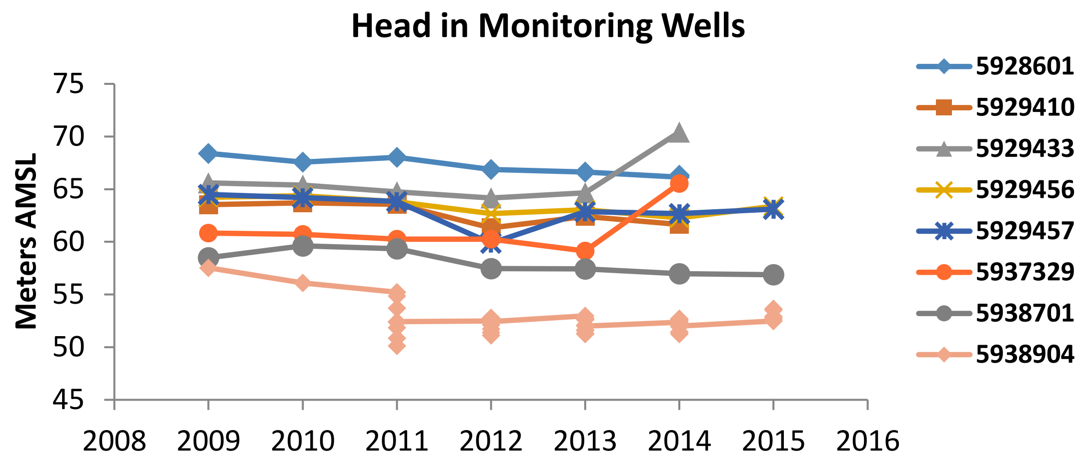

Figure 24. Measured head in monitoring well locations (data obtained from TWDB (2017))

Results and Discussion

Model Initialization

The coupled numerical model of the BRAA will be developed in stages, in order to maintain computational efficiency and to allow the model to converge easily while initializing the groundwater table and streamflow. In the first phase of model spin-up, a simple homogeneous subsurface will be simulated with no coupling to CLM. The initial depth to groundwater is specified by the user, and a steady-state recharge value is applied across the domain. The purpose of model spin-up is to apply steady-state boundary conditions until the model state reaches a dynamic equilibrium. This equilibrium point is typically defined when criteria such as unsaturated zone storage or mean depth-to-groundwater reach a consistent level of percent-change per timestep or per year (Ajami et al. 2014; Seck et al. 2015). So far, only preliminary tests of the numerical model have been completed to examine input files and to assess the model's ability to converge. Formal spin-up criteria for the BRAA model have not yet been defined. Future spin-up runs should start again from an initial state, with spin-up criteria already defined before running the model.

Preliminary tests showed that even though drainage of the domain toward a realistic mean depth-to-groundwater may take several months of simulation time, the model converges more easily when the entire domain is initially saturated (as opposed to setting an initial groundwater table several meters below the land surface). Starting from complete saturation allows a realistic soil moisture profile to develop in the unsaturated zone. In reality, the aquifer discharges only by baseflow to the river and pumping by irrigation wells. This version of the conceptual model is intended to be a baseline, pre-development scenario, so discharge is to the river alone. Then, the addition of wells in a future version can be compared to the baseline model to assess the effects of irrigation pumping on the Brazos River. These preliminary runs also used an internal boundary condition to generate steady-state streamflow at the upstream point. However, as described in the previous chapter, the ParFlow internal boundary condition option has behaved unpredictably and is not recommended for future use. Instead, the injection method is recommended.

Preliminary Model Runs

Preliminary tests of the numerical model were performed on the machines "Ada" and "Terra" at Texas A&M University's High Performance Research Computing resources, using a 14 x 14 x 1 parallel process topology (196 processors). Both homogeneous and heterogeneous runs were completed, for a few hours to a few days. No long-term simulations were attempted, as the groundwater table and streamflow have not been fully initialized. The preliminary runs were used to refine input files and to demonstrate that calculations for the complex domain geometry are indeed feasible.

For homogeneous runs with a timestep of 0.01 hour, computational efficiency varied from < 1.0 to 293 CPU-hours per model hour. (One CPU-hour is equivalent to one wall hour of parallel computing time on a single processor.) Run times for heterogeneous tests varied significantly due to the number of input configurations tested. Heterogeneous runs used an average of 261 CPU-hours per model hour, with a standard deviation of 363 CPU-hours.

Assumptions and Limitations

Grid Cell Size

Although a 100-m cell resolution is acceptable for land cover and subsurface processes, it can be a poor representation of a stream channel. ParFlow.CLM only permits variable cell sizes in the vertical direction, so reducing cell size near the river is not an option. This reach of the Brazos River has a variable width on the order of 100 m, so modeled discharge is expected to be fairly accurate. However, fine-scale changes in stage and inundated stream width are lost. This also affects the accuracy of modeled stream-aquifer exchanges. To improve modeled stream velocities, other studies (Bhaskar et al. 2015; Schalge et al. 2016) have recommended calibrating the Manning's roughness coefficient for cases in which the gridded river channel is much wider than in reality. Surface-groundwater exchanges could potentially be improved by modifying streambed porosity and permeability, but without fine-scale field measurements, exchange fluxes would be difficult to calibrate.

Surface Slopes

Rather than using a DEM directly, ParFlow requires input files of the surface slopes for each cell of the model grid. Although slopes are derived from the DEM, they undergo a significant amount of processing before being included in the model. Pits and flat spots are filled, but more importantly, the stream channels are artificially enforced using methods similar to those in other studies (Bhaskar 2010; Daniels et al. 2011). ArcGIS spatial analyst hydrology tools are used to delineate stream channels, and stream cells are then assigned the maximum slope values in the domain. This ensures that overland flow which reaches the stream stays in the stream and continues to the outlet, rather than getting stuck in a low spot or being accidentally routed sideways rather than downstream. However, the altered slopes will influence the channel velocities and subsequently the groundwater-stream exchanges.

Soils

The vertisols overlying much of the aquifer frequently shrink and create cracks, or macropores, that may act as preferential flow paths from the surface to the coarser alluvial materials. Chakka and Munster (1997) represented this macropore flow in a VS2DT model by creating simple pathways in the model grid which had high conductivity but low porosity. Artificially constructing macropores in this manner is infeasible for a cell size of 100 m. Preferential flow paths have been modeled in ParFlow for fractured tuff (Maxwell 2010) but not for cracking clay. ParFlow does not have any built-in tools for representing macropores. The optimized permeability for clay layers in the model is larger than typical values for clay, which allows an overall larger flux to pass through these layers.

Comparison to the TWDB GAM

A primary goal of this project is to compare the coupled ParFlow.CLM model to the MODFLOW Groundwater Availability Model. Both models offer advantages along with their own limitations. The GAM assesses the entire extent of the BRAA, while the coupled model is limited to two counties. The GAM also accounts for interactions with the upper portions of underlying aquifers. However, because the extent of our model is limited, most of the domain in the ParFlow.CLM model overlies clay and shale layers, so the exclusion of inter-aquifer exchanges is not unrealistic. The initial design for the ParFlow model does not account for well pumping or irrigation return flow, although this could be included in the future. One important advantage of the ParFlow.CLM model is that it incorporates multiple layers of five geologic materials and highly heterogeneous surface soil data, while the GAM subsurface is vertically homogeneous except for underlying formations. Additionally, the GAM is run at monthly and annual timesteps. The ParFlow.CLM model will be run at hourly timesteps with hourly forcing data so that the subsurface response to flood pulses can be studied.

Summary

A conceptual model has been presented for an integrated Earth systems model of the Brazos River Alluvium Aquifer in Brazos and Burleson Counties, Texas. The conceptual model incorporates land surface processes, shallow overland flow, and variably saturated subsurface flow in a fully-integrated modeling framework. The upward fining geologic profile is represented, as are scattered clay lenses and heterogeneous surface soils. The conceptualized model does not account for inter-aquifer exchanges with underlying formations. Its upstream and downstream boundaries are located based on the assumption that groundwater flow lines follow surface topography to the river. A method has been presented in a previous chapter for introducing transient streamflow at the upstream boundary on the same temporal scale as hourly meteorological forcing data.

The initial stages of development for the numerical model have also been described. Preliminary testing of the numerical model has demonstrated the need for considerable computational power. Many of the input files have been created and tested and are now available to begin spin-up. Some of the input files for the heterogeneous model need to be updated once data have been gathered for van Genuchten parameters. The BRAA domain has only been run in ParFlow; CLM has not yet been applied.

CHAPTER IV

CONCLUSIONS

ParFlow.CLM is an integrated surface-subsurface hydrological model that also incorporates land surface processes. It can be run on multiple processors in parallel, which makes it an ideal choice for many large and complex model domains. However, a lack in the model program has limited its use to headwater catchments. A method for introducing transient stream inflow at high frequency over long simulations has been developed, which expands the applicability of ParFlow.CLM.

Recommendations for Future Work

A conceptual model has been presented for an integrated Earth systems model of the Brazos River Alluvium Aquifer, and the numerical model is in development. The BRAA model incorporates the newly developed method for introducing transient stream inflow in a ParFlow.CLM domain. Subsurface hydraulic properties are based on available data, but will require calibration. However, calibration of Manning's roughness coefficient is recommended first, as surface flows are highly dependent on the interaction of this parameter and the defined topographic slopes and grid cell size.

One objective for the proposed numerical model is to assess the response of the BRAA to extreme events, such as the 2011 drought and recent periods of flooding. While most groundwater systems have long residence times and reflect a highly dampened response to surface conditions, the BRAA is shallow and highly connected to the river. Alden and Munster (1997) observed a strong relationship between river stage and both horizontal and vertical flow velocities in the BRAA. Wrobleski (1996) determined that the influence of the river on groundwater levels is indeed strong but decreases with increasing distance from the river, which was corroborated by Rhodes (2016). Future researchers can improve upon these observations by specifically modeling flood and drought periods in the integrated ParFlow.CLM framework. A deeper understanding of the aquifer's response to flooding and drought may give insight to water resource planners about how irrigation needs and groundwater availability are related in this system.

Additionally, comparisons to the GAM may provide insight to water resource planners. The purpose of designing a coupled Earth systems model for the alluvium aquifer was to better represent exchanges between each part of the water cycle instead of relying on long-term estimates for baseflow or recharge. The same goes for the Water Availability Model for the Brazos River Basin, which relies on channel loss factors to represent streamflow losses to groundwater and evapotranspiration (Wurbs 2011). Finally, this model is intended to support ongoing data collection in the Texas Water Observatory.

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