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Investigation of modern leakage based on numerical and geochemical modeling near a municipal well field in Memphis, Tennessee.

Khairul Hasan

INVESTIGATION OF MODERN LEAKAGE BASED ON NUMERICAL AND GEOCHEMICAL MODELING NEAR A MUNICIPAL WELL FIELD IN MEMPHIS, TENNESSEE.

By

Khairul Hasan

A Dissertation

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DEDICATION

This dissertation is dedicated to my three most important persons: my father, Abul Khair; my mother, Khairun Nesa; and my wife, Khayrun Nahar.

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PREFACE

This dissertation is presented in five chapters. Chapter 1 briefly introduces the background of numerical and geochemical modeling to investigate modern leakage. Chapter 2 documents the latest update and recalibration of an existing groundwater flow model in Shelby County. The chapter is formatted in the **Applied Water Science** journal style, to which it was submitted for publication. Chapter 3 describes the integrated hydrostratigraphic analysis, numerical modeling, hydrologic tracers, and geochemical modeling to identify the source(s) and pathways of modern water. Chapter 3 is formatted following the **Environmental Earth Sciences** journal style, to which it will be submitted for publication. The summary and conclusion of the research are outlined in Chapter 4. The references cited in this dissertation are listed in Chapter 5.

ABSTRACT

Local leakage processes and potential migration pathways of modern water (<60 years) from the shallow aquifer, into the underlying semiconfined Memphis aquifer, were evaluated to assess the vulnerability of groundwater in Memphis Light, Gas and Water's (MLGW) Sheahan well field. To identify the source(s) and pathways of modern water, integrated hydrostratigraphic analysis, numerical modeling, hydrologic tracers, and geochemical modeling were utilized. The percentage of modern water present in Memphis aquifer production wells is estimated using inverse geochemical modeling, lumped parameter modeling, and solute transport modeling with Modular Transport, 3-Dimensional, Multi-Species model (MT3DMS). The mixing percentages determined from lumped parameter modeling and MT3DMS are generally in agreement except well 87A, estimating up to 14.3% and 15.3%, respectively. The significant mixing fraction difference at 87A might account for the missing hydrogeologic connection in the groundwater model on the eastern part of the well field. Estimates for the apparent age of the modern water derived from MT3DMS fall within the age range obtained from environmental tracer data ($^{3}H/^{3}He$). However, the age distributions from the MT3DMS model are limited to 60 years or less, resulting in a younger mean age than the tracer-based apparent ages. Thus, the MT3DMS model, calibrated with long-term tracer data could simulate the mean age and mixing percentage of modern water while emphasizing the importance of accurate hydrogeologic conceptualizations at the Sheahan well field. As a result, tracer data and solute transport modeling can identify vulnerabilities and ensure the long-term sustainability of the Sheahan well field.

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INTRODUCTION

Throughout much of Shelby County, the Memphis aquifer is protected from downward leakage of lower-quality water by one or more relatively low permeability layers within the upper Claiborne confining unit (UCCU or aquitard) (Graham and Parks 1986; Parks 1990). Recent studies suggest that there are localized areas where clay intervals within the UCCU are either thin (< 3 m thick) or absent, creating preferential pathway zones termed “breaches,” causing local variability in inter-aquifer water exchange and potential for degradation of groundwater quality (Graham and Parks 1986; Larsen et al. 2003; Gentry et al. 2006b; Waldron et al. 2009, 2011; Carmichael et al. 2018; Torres-Uribe et al. 2021; Villalpando-Vizcaino et al. 2021). A better understanding of the recharge pathway of inter-aquifer flow through breaches is required for assessing the vulnerability and sustainability of a well field, which is often difficult to quantify. Identifying and characterizing aquitard breaches requires costly detailed subsurface geological investigations (Gentry et al. 2006a; Waldron et al. 2009; Jazaei et al. 2019).

Local groundwater flow models could adequately simulate these localized zones of higher hydraulic conductivity (breaches) within a complex hydrogeologic system in Shelby County (Torres-Uribe et al. 2021; Villalpando-Vizcaino et al. 2021). However, there are only a few groundwater models available for Shelby County, and several of these models (Arthur and Taylor 1990, 1998; Brahana and Broshears 2001; Clark and Hart 2009) did not account adequately for vertical leakage due to the absence or misrepresentation of the aquitard unit. Recently several numerical groundwater models (Jazaei et al. 2019; Torres-Uribe et al. 2021; Villalpando-Vizcaino et al. 2021) have been developed that can effectively simulate the semi-confined Memphis aquifer, which serves as a community’s water supply in urban areas such as Shelby County, Tennessee.

Additionally, the combined application of tracers and geochemical modeling has been used throughout the years to estimate and assess the modern water leakage (Larsen et al. 2003, 2016; Gentry et al. 2006b; Kingsbury et al. 2017). Age-dating tracers (^{3}H and ^{3}He) can identify production wells containing modern water and yield mean ages, which are evaluated against hydrogeologic data to identify potential leakage sources and pathways. Also, environmental tracers yield mixing percentages of modern water using lumped parameter modeling (LPM) that considers simplified aquifer settings and groundwater flow dynamics (Jurgens et al. 2012). On the other hand, geochemical modeling of water chemistry using the United States Geological Survey (USGS) PHREEQCi program has been used in several well fields in Shelby County, including Sheahan, to estimate the mixing percentage of shallow groundwater with Memphis aquifer water in the vicinity of production wells (Larsen et al. 2003, 2013; Koban et al. 2011).

This research presents a case study of integrated hydrostratigraphic analysis, numerical modeling, hydrologic tracers, and geochemical modeling to evaluate the local leakage process and potential migration pathways of modern water from the shallow aquifer to the underlying water supply aquifer.

GROUNDWATER FLOW SIMULATION

Introduction

Simulating the behavior of aquifer systems, evaluating aquifer parameters, and efficient groundwater management for the past, present, and future are the fundamental purposes of groundwater modeling (Zhou and Li 2011; Anderson et al. 2015; Omar et al. 2021). Throughout the years, groundwater flow models have become a valuable tool embraced by many hydrogeologists and researchers, as they can be used for many purposes, such as groundwater sustainability, and for informed decisions when it comes to groundwater management (Shuler and Mariner 2020; Omar et al. 2021). Since groundwater models are often plagued with parameter uncertainty and non-uniqueness, an adaptive management strategy based on iterative decision making should be considered to reduce the uncertainty over time (Anderson et al. 2015). Thus, models need to be periodically updated and refined with new data as it becomes available to improve the accuracy and reliability of the model (Anderson et al. 2015; Condon et al. 2021).

Likewise, a groundwater model is also an effective tool to simulate the inter-aquifer water exchange in groundwater systems comprised of leaky aquitards, which may pose a potential contamination threat due to the vertical hydraulic connections between the shallow and semi-confined aquifers. Recently several numerical groundwater models (Jazaei et al. 2019; Torres-Uribe et al. 2021; Villalpando-Vizcaino et al. 2021) have been developed that can effectively simulate the semi-confined Memphis aquifer, which serves as a community's water supply in urban areas such as Shelby County, Tennessee. Shelby County (Figure 1) is in the southwestern corner of Tennessee, and centrally located in the Mississippi embayment, a multi-state sedimentary basin hosting an aquifer system composed of alternating layers of sand, silt and clay (Hart and Clark 2008). Shelby County is underlain by three primary aquifers: the shallow, Memphis, and

Fort Pillow (Jazaei et al. 2019). Throughout much of Shelby County, the Memphis aquifer is protected from downward leakage of lower-quality water from the shallow aquifer by one or more relatively low permeability layers within the upper Claiborne confining unit (UCCU or aquitard) (Graham and Parks 1986; Parks 1990). Recent studies suggest that there are localized areas where clay intervals within the UCCU are either thin (< 3 m thick) or absent, creating preferential pathway zones termed “breaches,” causing local variability in inter-aquifer water exchange and potential for degradation of groundwater quality (Graham and Parks 1986; Larsen et al. 2003; Gentry et al. 2006b; Waldron et al. 2009, 2011; Carmichael et al. 2018; Torres-Uribe et al. 2021; Villalpando-Vizcaino et al. 2021). A better understanding of the recharge pathway of inter-aquifer flow through breaches is required for assessing the vulnerability and sustainability of a well field, which is often difficult to quantify. Local groundwater flow models could adequately simulate these localized zones of higher hydraulic conductivity (breaches) within a complex hydrogeologic system in Shelby County (Torres-Uribe et al. 2021; Villalpando-Vizcaino et al. 2021). However, there are only a few groundwater models available for Shelby County, and several of these models (Arthur and Taylor 1990, 1998; Brahana and Broshears 2001; Clark and Hart 2009) did not account adequately for vertical leakage due to the absence or misrepresentation of the aquitard unit.

Most recently, Villalpando-Vizcaino et al. (2021) developed a multi-layered, subregional groundwater model for Shelby County, also known as CAESER-I, to assess inter-aquifer water exchange between the shallow, Memphis, and Fort Pillow aquifers with their intervening confining units. Torres-Uribe et al. (2021) extended the CAESER-I model backward in time to January 1960 to assess the spatial configuration of breaches near the Sheahan well field, which is owned and operated by Memphis Light, Gas and Water (MLGW), the main utility company in the Shelby County area. By comparing simulated parameters against published age-dating and geochemistry data, Torres-Uribe et al. (2021) suggested the presence of a large and spatially extensive paleochannel as a breach within the Sheahan well field. But this paleochannel feature was formed by erosional and depositional processes of shallow aquifer material atop the UCCU, as Pell et al. (2005) suggested. Other limiting factors of Torres-Uribe et al. (2021) analysis were the uncertainty of breach hydraulic parameters, which required them to test breach vertical hydraulic conductivity (Kv) by varying it across three orders of magnitude; setting the shallow aquifer initial head constant; including only historical pumping data for MLGW well fields till 2016; and did not fully recalibrate the model with Parameter ESTimation (PEST).

Paul (2022) further modified the CAESER-I model to couple with a genetic algorithm to develop a well placement and pumping optimization strategy to ensure long-term production from MLGW's well fields, by constraining the migration of young water via inter-aquifer leakage through UCCU breaches. This study, however, utilized a modified breach geometry by Larsen et al. (2022) and a recurrent particle tracking method to determine the Kv value of the breach that permits particles to penetrate down the upper segment (top 100m) of the Memphis aquifer.

Jazaei et al. (2019) developed a localized numerical groundwater model (prior to CAESER-I) to identify possible leaky aquitard zones by targeting three MLGW well fields: Allen, Davis, and Palmer. The study identified five suspected breach zones using pilot-point calibration, velocity and flow budget, and particle tracking. Of these five leaky zones, three (zones 1, 2, and 4) were validated by previous studies (Parks and Carmichael 1990b; Carmichael et al. 2018).

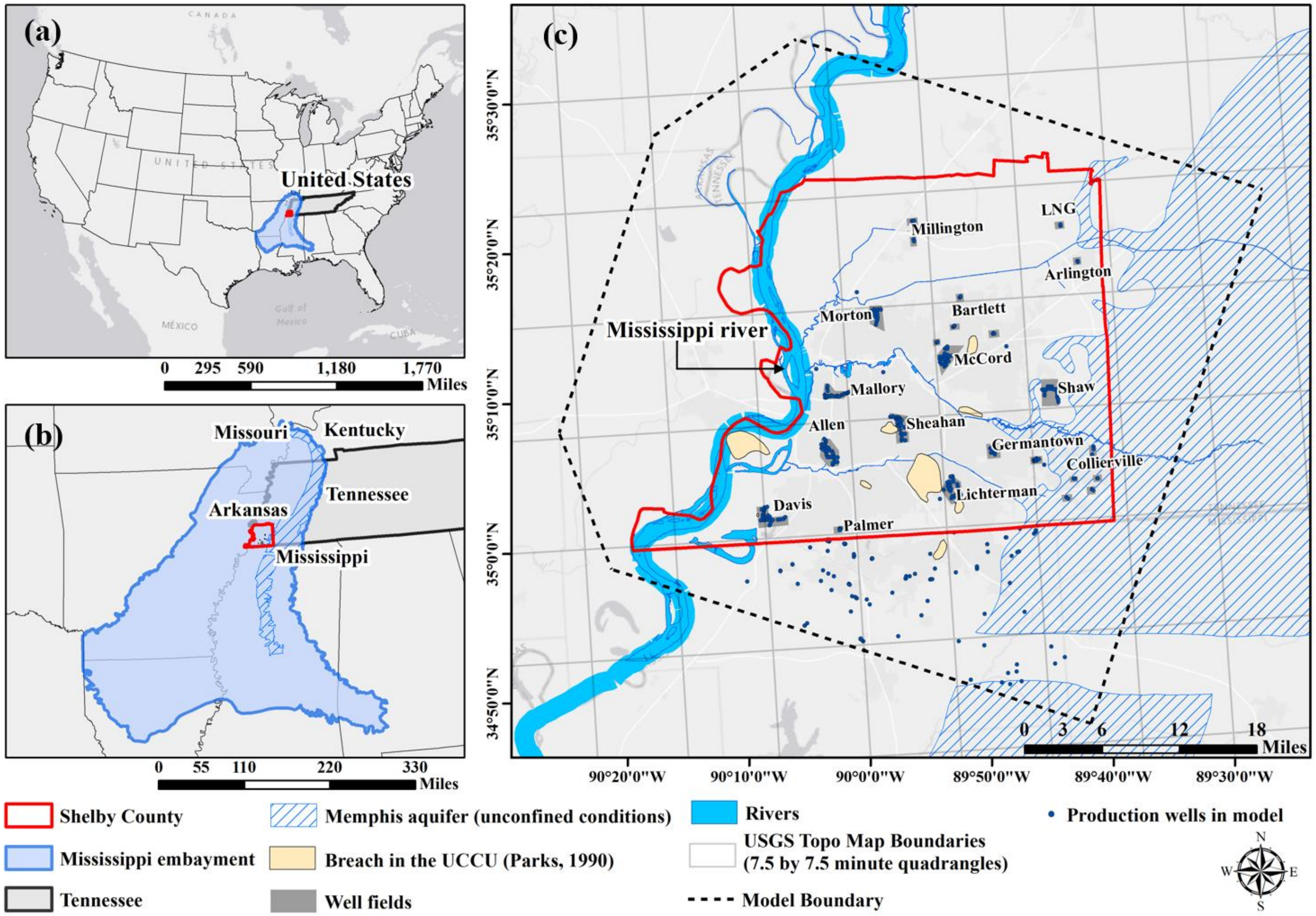

Figure 1. (a) Mississippi embayment aquifer system; (b) Location of Shelby County within the embayment. (c) Study area showing CAESER-I boundary, rivers, well fields, production wells (2021), interpreted breaches and Memphis aquifer unconfined zone by Parks (1990). Modified from Villalpando-Vizcaino et al. (2021).

In brief, the CAESER-I model simulated the inter-aquifer water exchange in the Shelby County area between all three primary aquifers: shallow, Memphis, and Fort Pillow, and the two confining units, the UCCU and Flour Island. It simulated individual well pumping monthly between January 2005 to December 2016, treated the shallow aquifer as variable head, and accounted for leakage through the UCCU. Even though the CAESER-I model was able to model aquitard breaches, their hydraulic properties were uncertain and derived from calibration using Parameter ESTimation (PEST), where Villalpando-Vizcaino et al. (2021) provided an average breach Kv of 1.4×10^{-4} for those breaches inferred by Parks (1990). Additionally, Paul (2022) estimated the breach Kv range as 5×10^{-4} to 4×10^{-3} m/day for breaches adjacent to Allen, Sheahan, Lichterman, McCord, and Davis well fields. Again, the investigation by Torres-Uribe et al. (2021) found Kv to be 0.1524 m/day for a single breach near the Sheahan well field by varying an order of magnitude higher and lower than Kv as defined by Gentry et al. (2006a).

In addition, CAESER-I and later updated versions (Torres-Uribe et al. 2021; Paul 2022) had limited measurements of hydraulic conductivity and storativity which may have resulted in non-unique solutions (Tian-chyi et al. 2015; Jazaei et al. 2019; Villalpando-Vizcaino et al. 2021; Sahagún-Covarrubias et al. 2022). Lastly, CAESER-I's stress periods spanned 2005 to 2016; however, when considering using CAESER-I for contaminant transport, the majority of contaminant sources in Shelby County originated after World War II (post 1945) prior to the Clean Water Act around 1972. Therefore, it was apparent that CAESER-I would require updating and recalibration to an early period (i.e., 1960 mentioned later).

This study documents the latest update and recalibration of the CAESER-I groundwater flow model. The modified model, CAESER-II, more accurately reflects the flow dynamics between all primary aquifers, aquitards and breaches in the Shelby County area, for an extended period of time and can be used to simulate contaminant transport from the time of sourcing, reevaluate inter-aquifer water exchange, and develop wellhead protection areas based on real historical pumping rather than estimations.

Model overview and modification

Regional hydrogeology

Villalpando-Vizcaino et al. (2021) provided a comprehensive overview of the hydrogeology of Shelby County. The shallow aquifer, UCCU, Memphis aquifer, Flour Island confining unit, Fort Pillow aquifer, and the Old Breastworks confining unit make up the first 500m of subsurface in Shelby County (Figure 2) (Villalpando-Vizcaino et al. 2021). The shallow aquifer (east of the Mississippi River bluff) consists primarily of sand and gravel with a typical horizontal hydraulic conductivity range of 1.5 to 45 m/day and is overlain by a surficial unit of silt or loess (Graham and Parks 1986; Parks 1990; Van Arsdale et al. 2007; Torres-Uribe et al. 2021). The UCCU confines most of the underlying Memphis aquifer and protects it from pollution, except in locations where breaches exist. The UCCU unit is composed of clay, silt, and sand, varying in thickness from 0 to 110 m, thinning toward the eastern part of Shelby County (Graham and Parks 1986). The vertical hydraulic conductivity of the UCCU varies between 1.5×10^{-6} to 3.0×10^{-4} m/day (Robinson et al. 1997). The only measured value of a UCCU breach hydraulic conductivity using falling head slug test at Shelby Farms was 0.1524 m/day (Gentry et al. 2006a; Torres-Uribe et al. 2021). The Memphis aquifer, a sand-dominated aquifer, supplies the majority of water used in Memphis and western Tennessee (Parks and Carmichael 1990b). It has a thickness of 150 to 270 m becoming unconfined in east-southeast Shelby County and an average hydraulic conductivity of 15 m/day with storage coefficients ranging from 0.003 to 0.01

m^{-1} (Parks and Carmichael 1990b; Waldron et al. 2011; Villalpando-Vizcaino et al. 2021). The Flour Island confining unit is 49 to 94 meters thick and separates the Memphis and fine- to medium-grained sand Fort Pillow aquifers (Parks and Carmichael 1989).

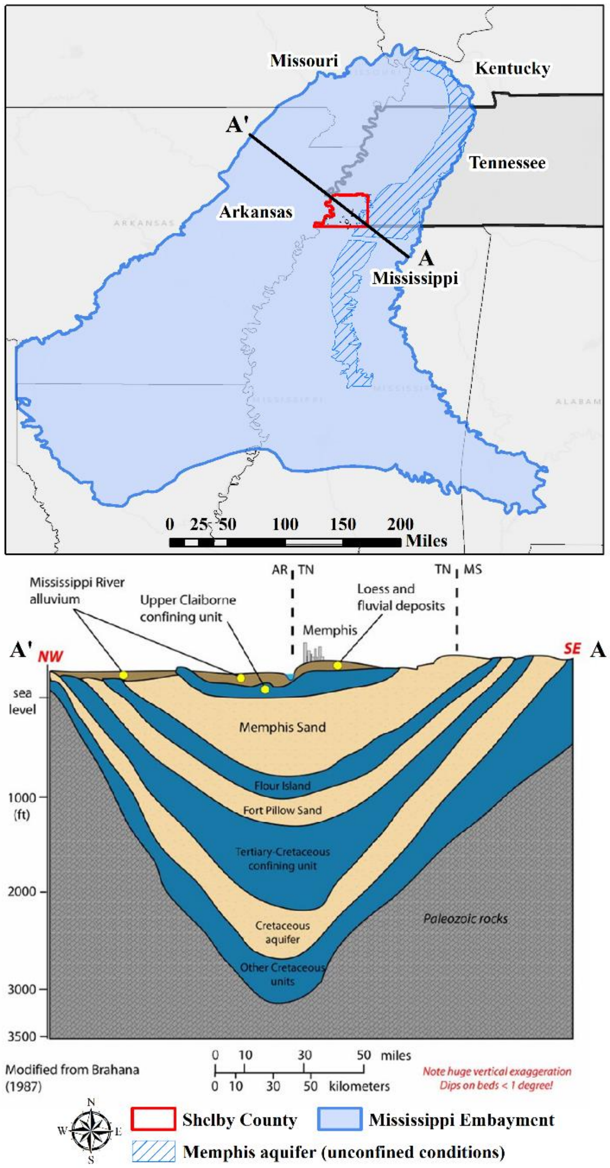

Figure 2. Mississippi embayment aquifer system (Clark and Hart, 2009) with a northwest to southeast generalized hydrologic cross-section A-A′ of the groundwater system beneath Memphis, Tennessee (modified from Brahana 1987; Brahana and Broshears, 2001), including four aquifers and confining units, across the Mississippi embayment. Additional units below the Fort Pillow are not part of this study.

In general, the CAESER-II model retains a similar conceptualization as the previous version (CAESER-I). The CAESER-I model was developed using the United States Geological Survey (USGS) MODFLOW-NWT program (Niswonger et al. 2011) which addresses dry cells issues, such as those caused by groundwater draining via breaches. Figure 1 shows the location of the CAESER-I model domain. Each grid cell inside the model domain has a uniform horizontal dimension of 250 m to accommodate a single well and avoid pumping over-lumping. The CAESER-I model consists of eight layers, with Layer-1 representing the shallow aquifer, Layer-2 being the UCCU with aquitard breaches, Layers 3 to 6 representing the Memphis aquifer, Layer 7 representing the Flour Island and Layer-8 being the Fort Pillow aquifer. Typically, each layer corresponds to one hydrogeologic unit, but the Memphis aquifer was divided into four layers to ensure a greater percentage of production wells (72%) have at least 80% of their well screen within a single layer (Villalpando-Vizcaino et al. 2021).

Boundary conditions

Following Villalpando-Vizcaino et al. (2021), the upper boundary of the model is the water table, whereas the lower boundary is the Old Breastworks confining unit, which is treated as no-flow boundary following modeling by Brahana and Broshears (2001) and Clark and Hart (2009). The shallow aquifer is bounded to the west by the Mississippi River (Figure 3) and has specified heads defining its eastern extent.

In CAESER-I, the Memphis aquifer is bounded by constant head boundaries to the east and at the southwest corner, consistent with historical water levels Schrader (2007) in nearby wells Fa:R-002, Ar:H-002 and Ar:C-001 for the 2005-2016 period (Figure 3). Based on extended available data for these wells from the USGS National Water Information System (NWIS)

(Figure 4), constant head boundaries were left with the values set in CAESER-I, as levels for the 1960-2021 indicate average annual deviations of approximately 30 cm for Fa:R-002 and less than 1 m for Ar:H-002 and Ar:C-001.

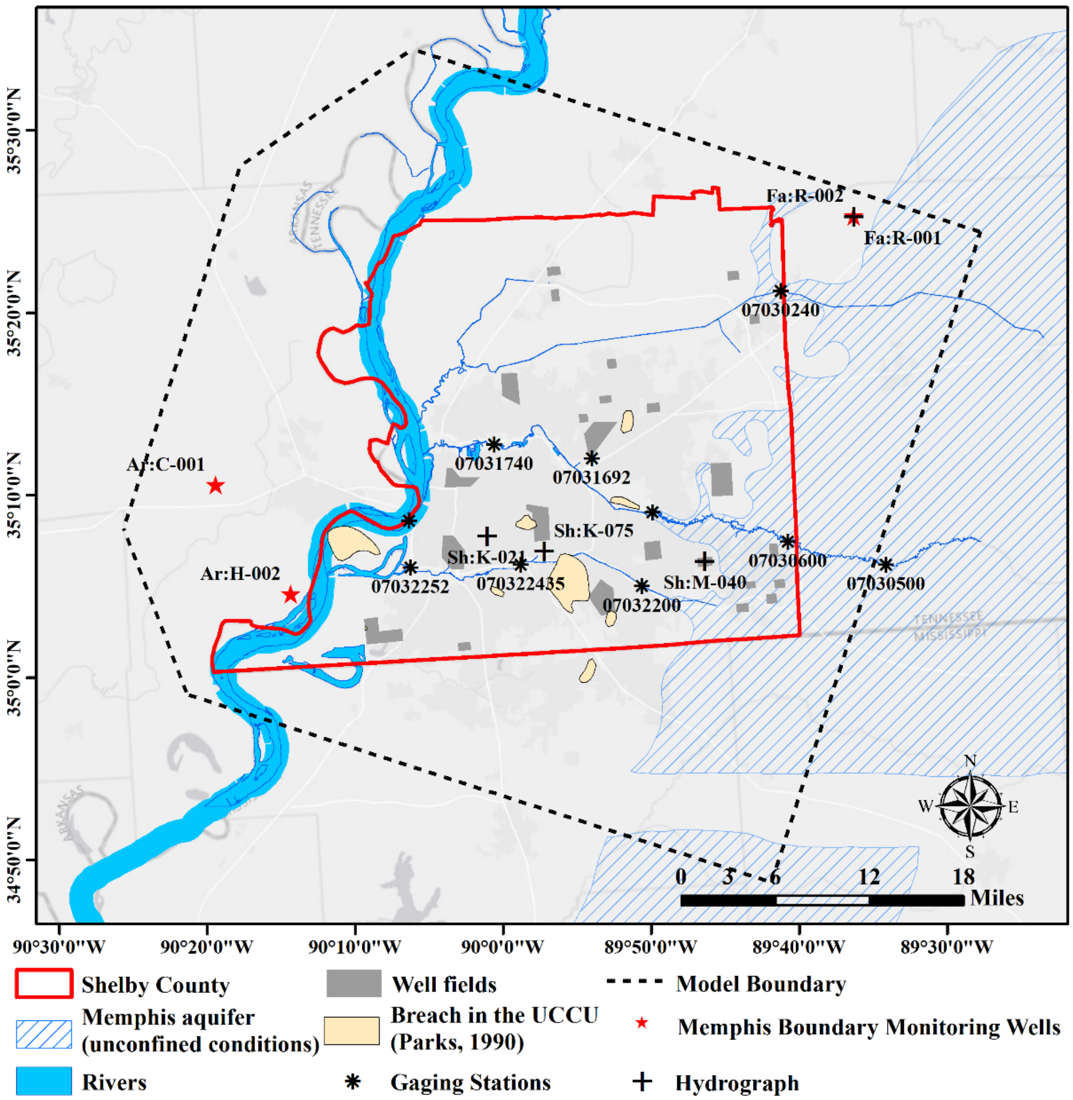

Figure 3. Monitoring wells and stream gauging locations in CAESER-II model. Red stars are the monitoring wells used for Memphis aquifer boundary selection. Black + markers are monitoring wells used for hydrograph analysis.

Because hydrologic gradients are parallel to the model boundaries, all remaining boundaries are modeled as no-flow, including the Fort Pillow aquifer as described by Villalpando-Vizcaino et al. (2021).

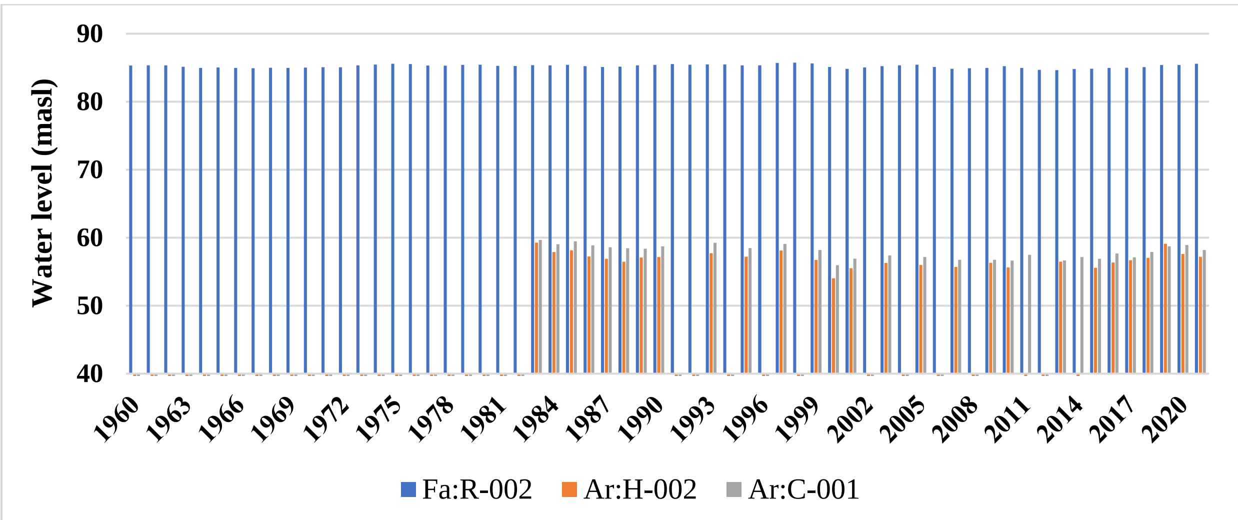

Figure 4. The historical water levels (masl) for monitoring wells in the Memphis aquifer between 1960 and 2021. Here, Fa:R-002 is located on the eastern boundary while Ar:C-001 and Ar:H-002 is located near the southwestern boundary.

Initial conditions

The initial conditions of the shallow, Memphis, and Fort-Pillow aquifers were adjusted in CAESER II for 1960 water levels. Due to a lack of data, it was difficult to model the transient water table as far back as 1960. The oldest available water-table map was constructed for fall 1988 (Parks 1990; Torres-Uribe et al. 2021) but makes an assumption that some of its water levels dating back to the 1940’s remained unchanged over time (such as USGS 7.5-minute quadrangles showing intersection of ground elevation contours with streams to represent water table elevations). Nonetheless, the starting head of the shallow aquifer was adjusted using water levels from six monitoring wells (Sh:K-075, Sh:P-099, Sh:R-032, Sh:Q-094, Sh:J-172, and Sh:J-171); all of which have historical data from 1987 and earlier. Following the trends in the monitoring well data, the water levels in 1960 were calculated by extrapolating head values at the observation wells backward to 1960. The spline interpolation method was then utilized to generate a smooth surface (Figure 5(a)) for 1960, beginning with fall 2005 water levels (Konduro-Narsimha, 2007) and holding the 1960 water level at the six monitoring wells constant.

The USGS 1960 Memphis aquifer potentiometric map was used for the Memphis aquifer starting head (Criner and Parks 1976). Similar to the shallow aquifer, initial heads for the Fort Pillow were derived from observation wells 11N08E10AAC2, **Sh:U-001**, **Fa:R-001**, **Sh:K-045**, **Sh:O-170**, 05N07E29ACC1, 09N08E29ADD1, and Sh:Q-154. Data for these observation wells either existed (bolded above) or were extrapolated backward to 1960, then a smooth surface was produced using the 1970 Fort Pillow potentiometric map by Criner and Parks (1976) (Figure 5(b)).

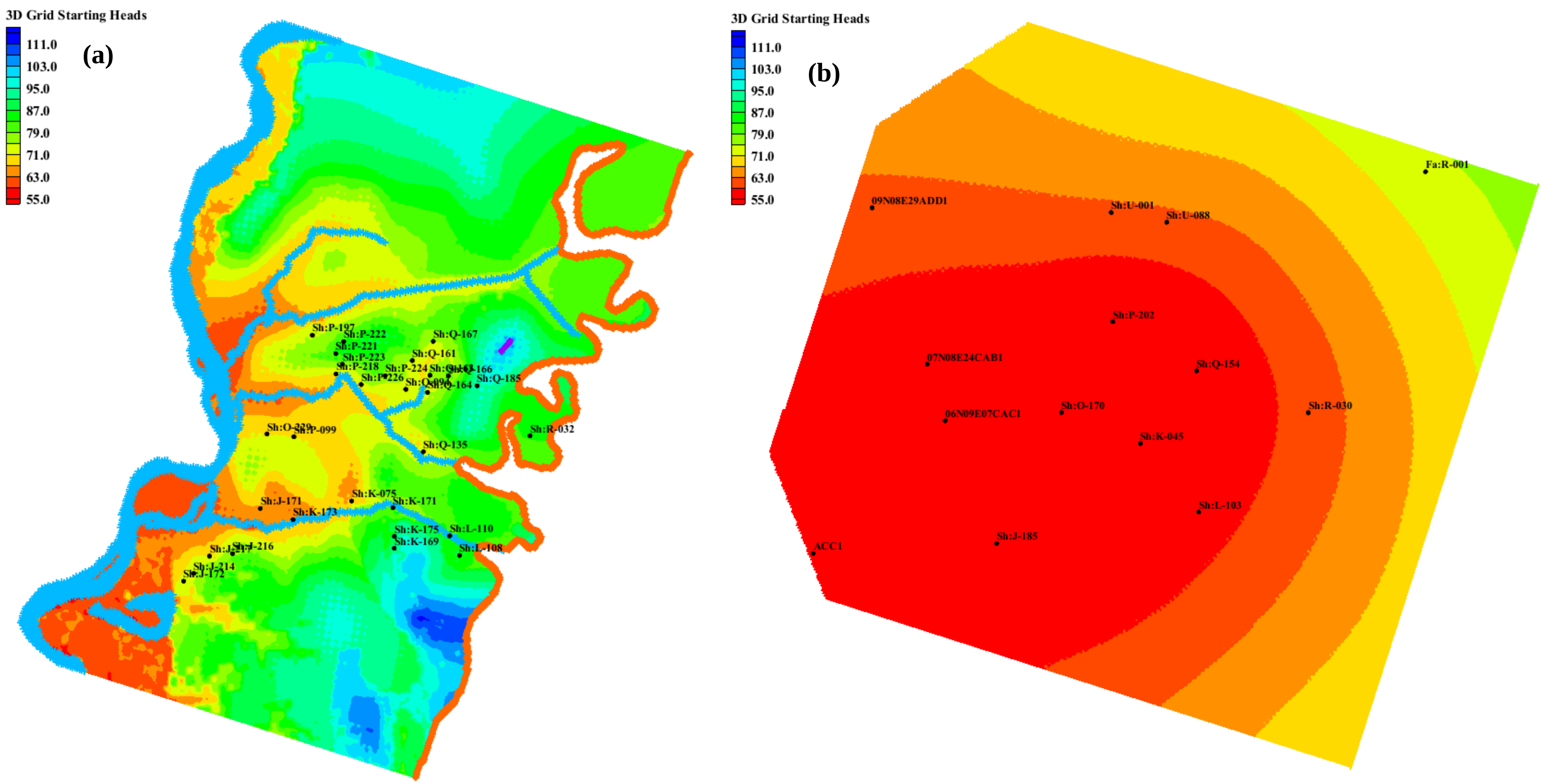

Figure 5. Interpolated starting heads for the shallow (a) and Fort Pillow (b) aquifers in 1960. Black dots represent monitoring wells providing control.

Hydraulic properties and recharge

Hydraulic conductivity and storativity for each hydrogeologic unit were initialized from the CAESER-I model. To improve against CAESER-I's non-uniqueness and uncertainty, CAESER-II incorporated recently measured hydraulic properties of the Memphis aquifer by (Sahagún-Covarrubias et al. 2022), as previously published literature values relied upon by CAESER-I were unreliable due to a wide range and low score on the scoring matrix developed by (Waldron et al. 2011), or derived during model calibration (Brahana and Broshears 2001; Clark and Hart 2009). The horizontal hydraulic conductivity (h_k) for the Memphis aquifer (Table 1) was calculated using pumping test data evaluated using Hantush and Jacob's (1955) equation for leaky confining Memphis aquifer (Sahagún-Covarrubias et al. 2022).

Table 1. Transmissivity, horizontal hydraulic conductivity and storativity values for the Memphis aquifer at different well fields (Sahagún-Covarrubias et al. 2022).

Well field	Observation Well	Transmissivity (m^2/day)	h_k (m/day)	Storativity
Sheahan	Sh:K-066	1,600	7.62	0.0007
	MLGW-72A	1,500	7.14	0.0005
Morton	Sh:P-113	3,100	14.76	0.0090
Germantown	Sh:L-089	2,500	11.90	0.0020
Davis	Sh:J-140	2,700	12.86	0.0010
	MLGW-401	2,800	13.33	0.0020
Mallory	Sh:O-211	1,800	8.57	--
	Sh:O-212	600	2.86	0.0020
	MLGW-016C	900	4.29	0.0006

Specific yield and vertical anisotropy ratio were left unchanged with 0.25 and 0.1, respectively; similarly, recharge rate values ranging from 1 to 8 cm/year were left to the model's top layer which represents the shallow aquifer and an unconfined section of Memphis aquifer (eastern Shelby County) (Villalpando-Vizcaino et al. 2021) as no new data had been produced to better inform CAESER-II.

Aquitard breaches

Parks (1990) approximated the spatial configuration of breaches using borehole logs and water level data, which has been widely used for the vulnerability assessment of Memphis aquifer. Nevertheless, a recent compilation of geophysical log data (Murphy 2017) and water-table surveys (Konduro-Narsimha 2007; Ogletree 2017) in Shelby County revealed that uncertainty exists in breach configuration and locations; therefore, further update/refinement is required at local scales.

Identification of localized, suspected breaches requires detailed subsurface geological and geochemical investigations, including well log data indicating an absence or thinning of clay intervals within the UCCU, anomalous water-table depressions, and/or evidence of modern water (Graham and Parks 1986; Parks 1990; Bradley 1991; Larsen et al. 2003, 2013, 2016; Gentry et al. 2006a; Konduro-Narsimha 2007; Ivey et al. 2008; Waldron et al. 2009; Bradshaw 2011; Koban et al. 2011; Ogletree 2017; Lozano-Medina 2022). Verification of any suspected breach requires drilling. But, due to the irregular distribution of high-resolution data, it is difficult to verify and constrain the shape of individual breaches throughout Shelby County, such as the Park (1990) breach near the Sheahan well field.

Breach identification at Sheahan well field

MLGW's Sheahan well field (Figure 6) was selected to identify new confirmed/suspected breach locations since this well field is best understood hydrogeologically and is constrained by high-quality well log data (Murphy 2017). In addition, previous research (Larsen et al. 2003, 2016; Gentry et al. 2006b; Ivey et al. 2008; Torres-Uribe et al. 2021) has attempted to evaluate the presence and extent of additional breaches beyond Parks (1990). Torres-Uribe et al. (2021)

suggested the presence of a large and spatially extensive paleochannel (i.e., breach) formed by erosional, depositional processes of the shallow aquifer material atop the UCCU (Figure 6). Hence, a contour map of the aggregate thickness of clay within UCCU was created using geophysical logs (Figure 6). A minimum thickness of 3 m of clay (Parks 1990) was used to identify suspected breach locations. Figure 6 illustrates the presence of three breaches within the UCCU at the Sheahan well field instead of the breach delineated by Parks (1990). The breaches in the central and western parts of the well field were verified by additional drilling and thus further refine the likelihood of a large paleochannel structure suggested by Torres-Uribe et al. (2021).

In addition, water level measurements were taken from shallow and Memphis aquifer monitoring wells in July 2020 in and around the Sheahan well field. The water-table surface showed an anomalous depression on the west side of the Sheahan well field around well Sh:K-163 (99s), which matches a previous study by Larsen et al. (2013) and later shown in Lozano-Medina (2022). No extensive withdrawals are known to occur from the shallow aquifer in this area that could result in water level depressions. Additionally, Memphis aquifer heads are lower than the water table, suggesting downward vertical leakage, a pattern also seen elsewhere in Shelby County (Bradley 1991; Carmichael et al. 1997; Konduro-Narsimha 2007; Ogletree 2017; Smith 2018).

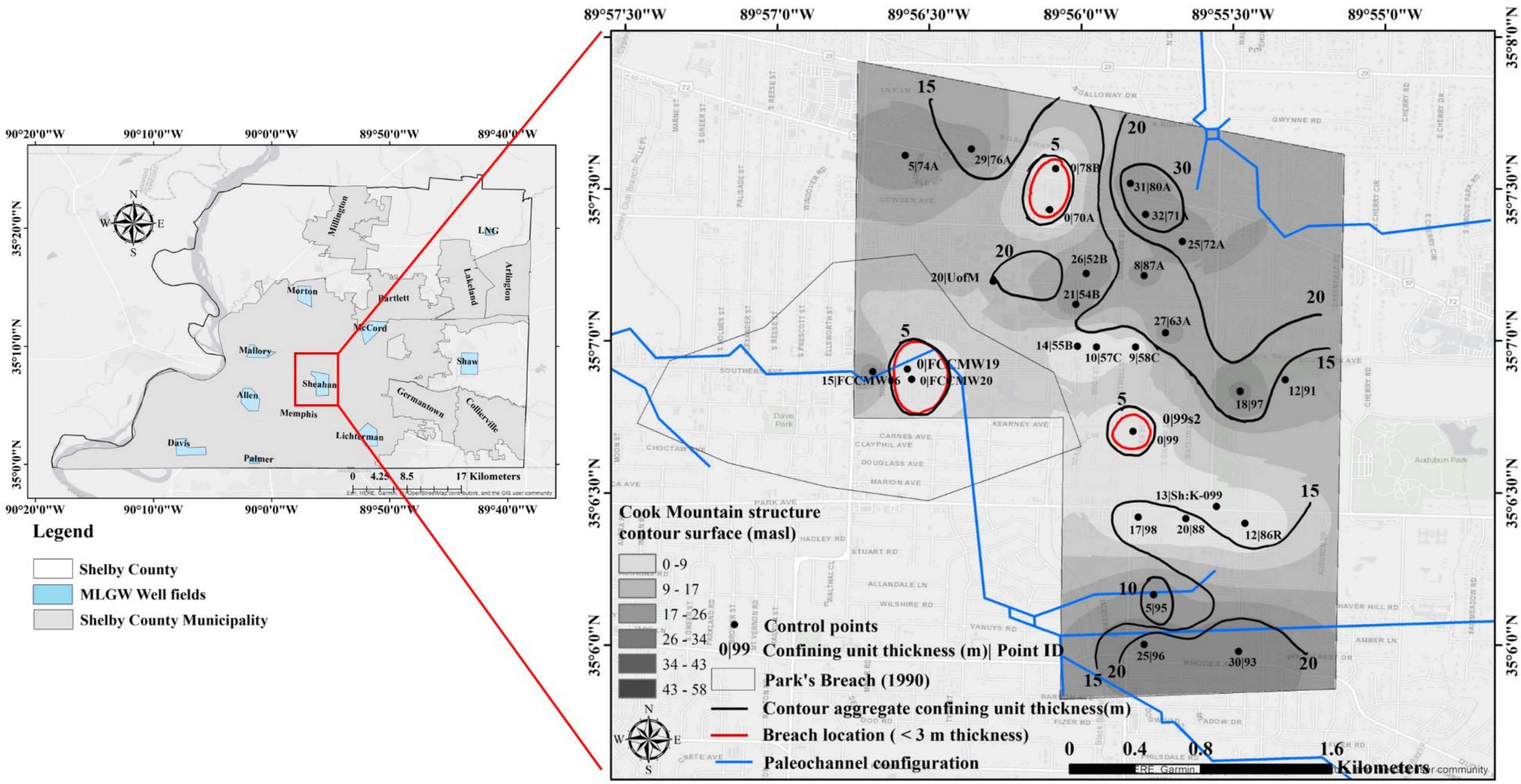

Figure 6. Contour map illustrating the aggregate thickness of confining clay within the UCCU. Thinned areas represent potential Cockfield paleochannels incised into and, in some areas, completely eroding the Cook Mountain Formation.

Moreover, water level data were collected every 15 minutes using Solinst Levelogger (Model 3001) pressure transducers (May 2019-November 2022) from the two shallow aquifer monitoring wells Sh:K-156 (96s) and Sh:K-163 (99s) and one Memphis aquifer monitoring well Sh:K-003 (UofM) using non-vented pressure transducers (data needs to be compensated against barometric pressure). Water level data were also obtained from the USGS National Water Information System (NWIS) database for the Memphis aquifer monitoring well, Sh:K-066. Water levels from monitoring wells are shown in Figure 7 and indicate that Memphis aquifer wells Sh:K-003 (UofM) and Sh:K-066 follow expected similar seasonal patterns responding to pumping stressors. In the case of the shallow aquifer, the general gradient of the shallow aquifer under Sheahan would tend to go south towards Nonconnah Creek, but instead, a pronounced lateral gradient is present going from the creek towards the well field and Sh:K-163 (99s) (Konduro-Narsimha 2007; Ogletree 2017; Lozano-Medina 2022). Adding to this general trend observed with discrete data, continuous data shows that groundwater levels in Sh:K-156 (96s) are higher than Sh:K-163 (99s); interestingly, the later mimics the seasonal patterns observed in the Memphis aquifer monitoring wells, something considered as an unexpected shallow aquifer response and more of an aquitard breach response (Villalpando-Vizcaino and Ledesma 2023). Similarly, and even though not as pronounced, Sh:K-156 (96s) seems to present a muted Memphis aquifer mimic response. Therefore, the general recharge mechanism in Sheahan well field is water from Nonconnah Creek travels along the paleochannel within the shallow aquifer toward the Sheahan well field before leaking into the Memphis aquifer through these breach locations shown in Figure 6.

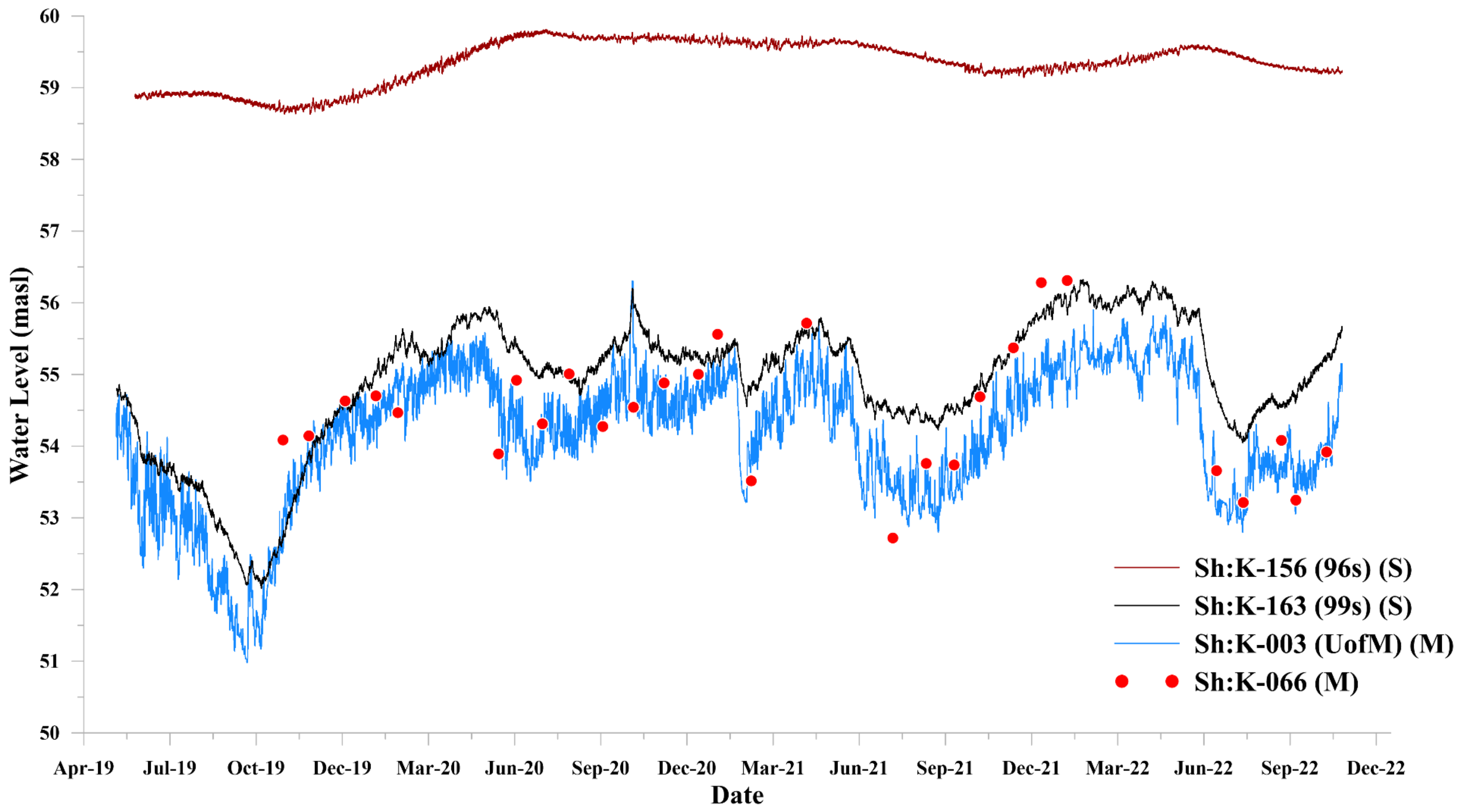

Figure 7. Plot of water levels for select monitoring wells in the Sheahan well field where (S) and (M) represent wells screened in the shallow (S) aquifer or Memphis (M) aquifer, respectively. Monitoring wells locations are shown in Figure 8.

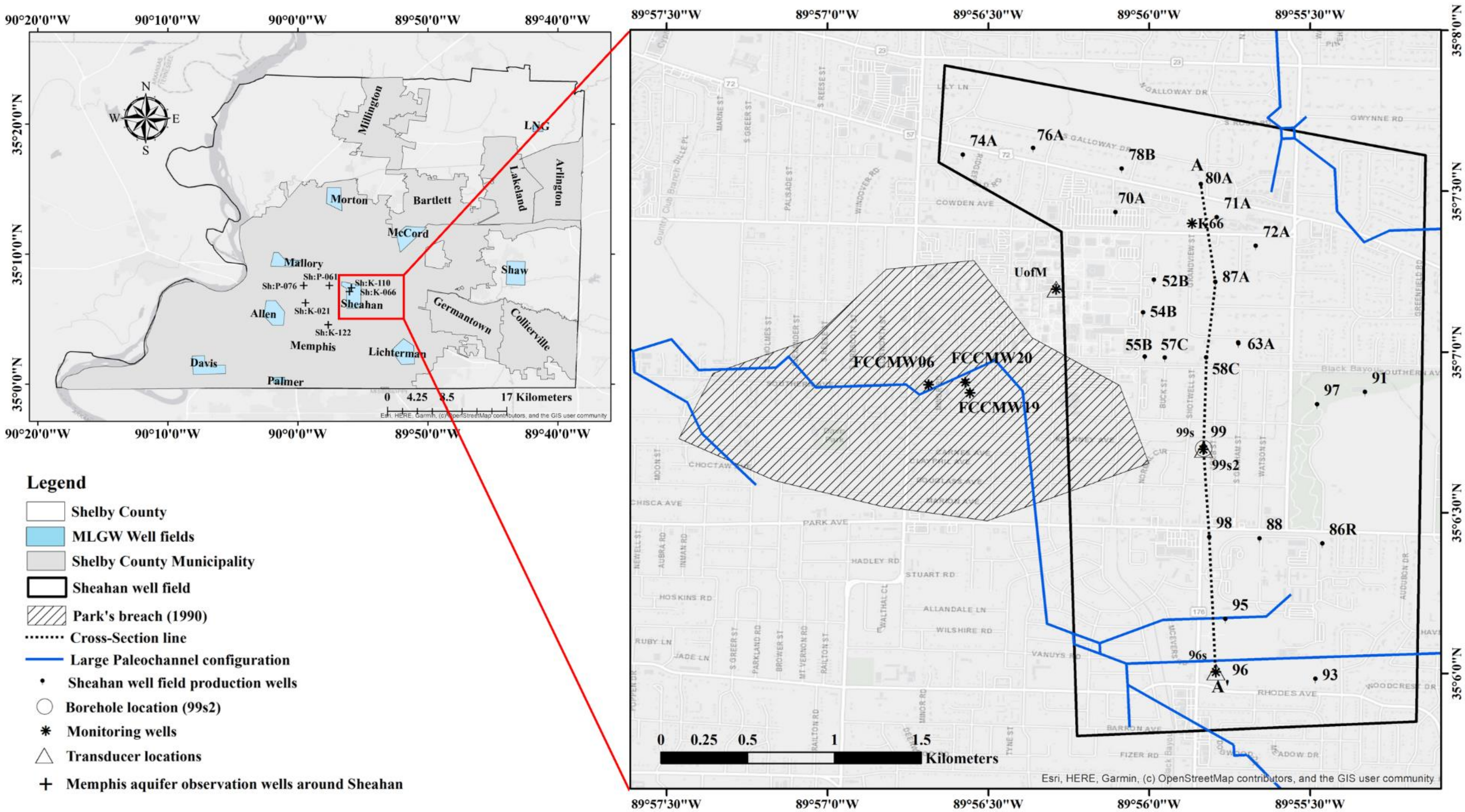

Figure 8. Layout of MLGW well fields and municipalities in Shelby County. Also shown is the newly drilled borehole 99S2, Parks (1990) breach, the large paleochannel breach, a Memphis aquifer monitoring well (Sh:K-066), Memphis aquifer observation wells around Sheahan, pressure transducer locations at the Sheahan well field and breach at Shelby Farms.

Rotasonic drilling and geophysical logging

The potential breach site around Sh:K-163 (99s) was selected for this study on the basis of thinning or absence of clay confining unit (Figure 6), anomalous water-table depression, and similar water level fluctuations as the Memphis aquifer (Figure 7). In January of 2021, a borehole named "99s2" was drilled next to observation well Sh:K-163 (99s) (Figure 8), using the sonic drilling technique for the purpose of capturing a continuous core that were analyzed for its geologic characteristics and engineering properties. The original observation well on site, Sh:K-163 (99s) has a depth of 47.6 m below ground surface (bgs), which is too shallow to confirm whether any portion of the UCCU exists further below. Hence, borehole 99s2 was drilled to a depth of 83.5 m bgs to fully penetrate the UCCU and be unquestionably within the Memphis aquifer, as shown in borehole log (Figures 9) and hydrogeologic cross-section (Figure 10). Borehole 99s2 is located on the same property lot as Sh:K-163 (99s) and production well MLGW-99, with a lot area at 1845 m^2. Continuous core samples were retrieved using a 10 cm diameter sampler and bagged at 3 m intervals during the drilling operation. Characterization of the sedimentary deposits, such as classification of the texture, color, and grain size, was conducted by splitting the core lengthwise following a procedure recommended by Alexander et al. (2011). Six representative samples were extracted at specific depths to determine hydraulic conductivity in the laboratory. The six depths were chosen based on changes in lithology and, therefore, taken at approximate depths of 20, 32.5, 53.5, 70, 72.5, and 77.5 m.

In the completed borehole, a Mount Sopris 40 GRP model geophysical wireline logging tool was lowered into the borehole to obtain a gamma response from the sedimentary deposits. Since the borehole was cased with steel pipe, resistivity and spontaneous-potential logs could not be obtained. The gamma log (Figure 9) obtained for 99s2 was correlated with geophysical logs from nearby production well and test boreholes in the Sheahan well field to construct a north-south stratigraphic cross-section through the middle of the well field (Figure 10). The cross-section indicates that at borehole 99s2, less than 10 m of silty-clay Pleistocene loess is underlain by Pliocene–Pleistocene sand and gravel fluvial-terrace deposit of the shallow aquifer, which extends to a depth of approximately 30.5 m. The fluvial-terrace deposits disconformably overlie sand and intraformational conglomerate of the Eocene Cockfield Formation, which disconformably overlies sand and clay of the Eocene Memphis Sand. The clay-rich Cook Mountain Formation is absent at borehole 99s2 and inferred to be absent at two adjacent boreholes (99 and 99s), indicating no continuous confining unit exists locally and, hence, represents a hydrogeologic breach.

Breach characterization

The gamma log obtained for 99s2 in concert with cross-section A-A′ indicates that samples taken at depths of 32.5 (Sample-2) and 53.5 (Sample-3) are within a breach in the UCCU. For these samples, saturated hydraulic conductivity was obtained using the falling head permeameter test following the ASTM D5856-15 and reducing the values 2.6 times due to account for disturbed soil conditions (Fenta et al. 2019). The samples were prepared at maximum dry density following equation described by Arvelo (2004). After reduction, the average vertical hydraulic conductivity obtained from the falling head permeameter test was 0.06 m/day (Table 2). The average hydraulic conductivity from grain-size analysis and the Kozney-Carman (1953) equation (Carrier III 2003) was 0.24 m/day (Table 2). The hydraulic conductivity from grain-size analysis based on empirical formulas often gives an order of magnitude higher estimate than permeameter test (Judge 2013). A slug test at nearby well, 99s, had hydraulic conductivity <0.15 m/d (horizontal) by Larsen et al. (2013) and Torres-Uribe et al. (2021) reported a model-derived vertical hydraulic conductivity 0.1524 m/day at this location.

Table 2. Hydraulic conductivity obtained from the falling head permeameter test and grain-size analysis.

	Hydraulic conductivity (Kozney-Carman 1953)	**Average hydraulic conductivity (m/day)**	**Kv (m/day) (Falling head test)**	**Average Kv/RF (m/day)**	**USCS classification**
Sample-2	0.36	0.24	0.13	0.06	Poorly graded sand with Silt (SP-SM)
Sample-3	0.12		0.17		Poorly graded sand with Silt (SP-SM)

* USCS = Unified Soil Classification System; RF = Reduction factor (2.6)

The hydraulic conductivity of all published breaches (Parks 1990) and three additional breaches at the Sheahan well field (Figure 5) were assigned to the model as initial value with the soil analysis for 99s2.

Rivers and streams

CAESER-II updated monthly input stages to the Mississippi River and its tributaries, the Wolf River, Loosahatchie River, and Nonconnah Creek within the MODFLOW (RIV) package; however, actual river stages were not available back to 1960 for all rivers except the Mississippi River. Also, month-by-month average stage fluctuations between years was less than 2 m for the majority of the gaging stations (Figure 3). Therefore, monthly mean river stages were obtained for the period 2005-2020 and repeated backward at 16-year intervals (CAESER-I timespan) to January 1960 following the methodology by Torres-Uribe et al. (2021). As no new measures of riverbed conductivity or thickness were available, the conductivity values from CAESER-I were used.

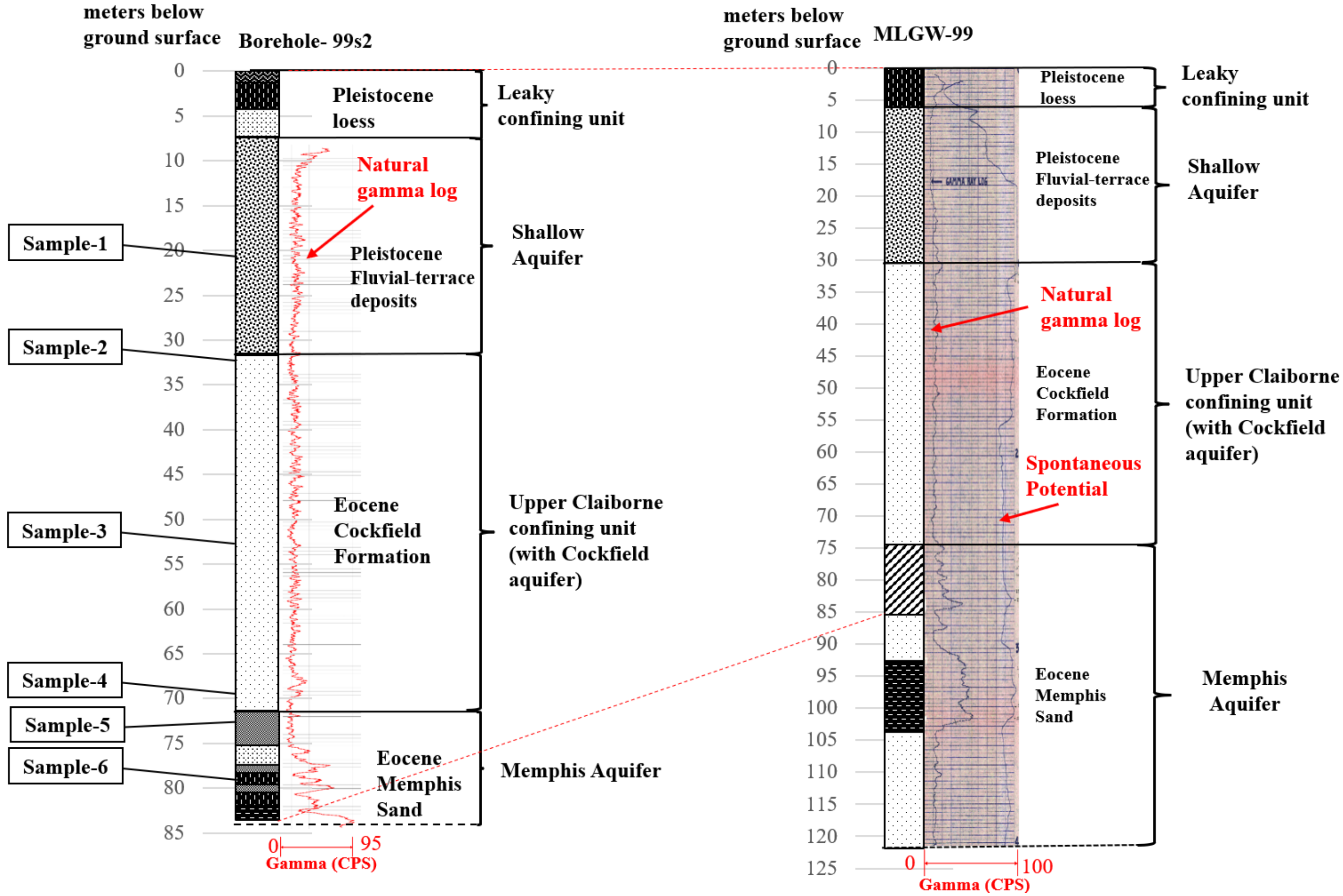

Figure 9. Interpretation of borehole-99s2 and MLGW production well 99 based on geophysical log showing principal geological and hydrostratigraphic units. The lithologic legend is same as in Figure 10.

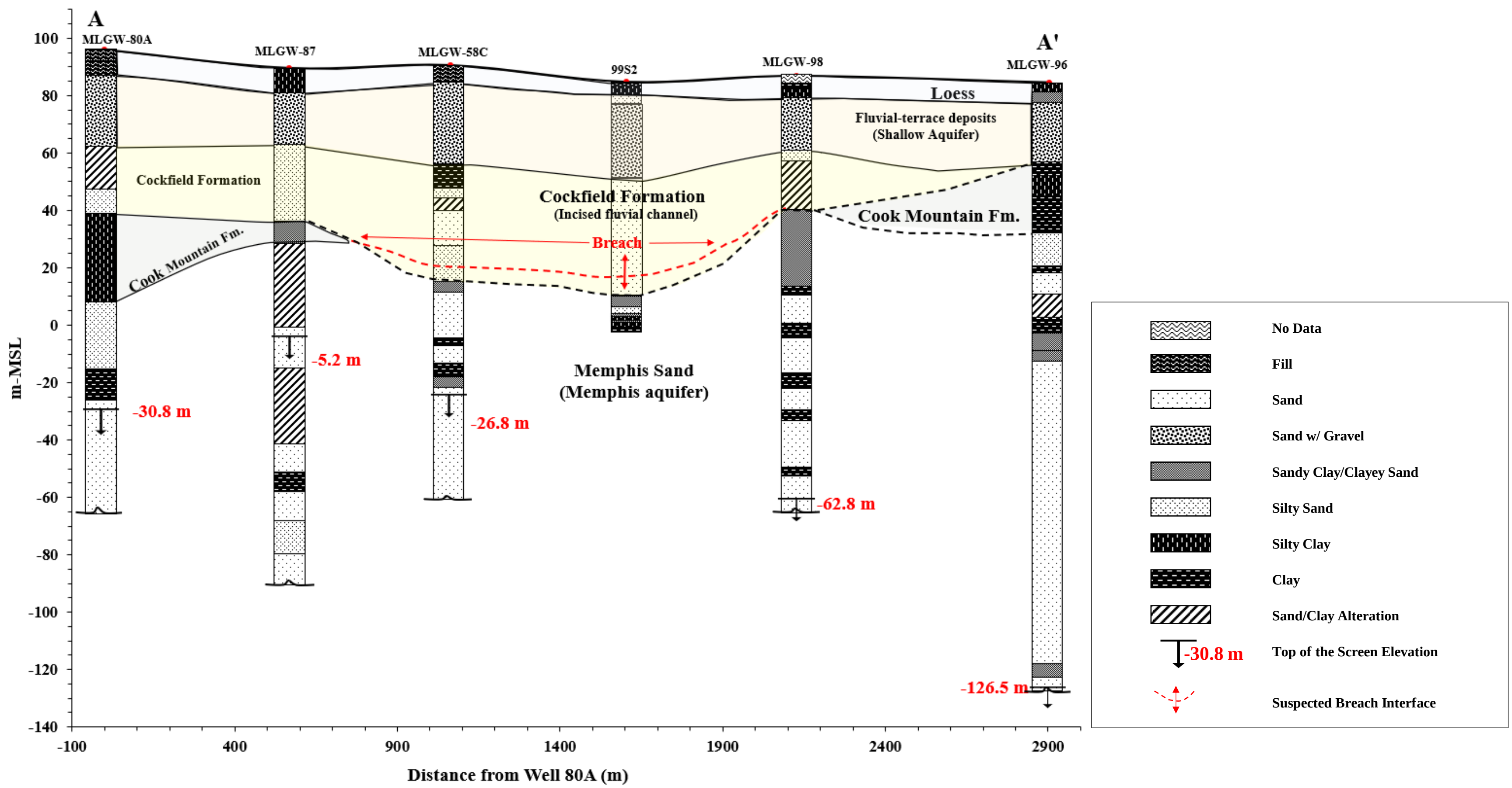

Figure 10. North-south stratigraphic cross-section A-A′, Sheahan well field. Location of cross-section A-A′ is shown on Figure 8.

Wells and groundwater withdrawal

The CAESER-II model includes 345 high-capacity production wells at depths ranging from 30 to 301 meters in the Memphis aquifer and 350 to 470 meters in the Fort Pillow aquifer. In contrast, CAESER-I model had 336 production wells with historical data from 2005 to 2016. In addition, Torres-Uribe et al. (2021) incorporated historical pumping data for only MLGW well fields from 1960 to 2016 for CASER-I wells; hence, this investigation also added historical industrial pumping. Similar to the CAESER-I model, the CAESER II model considered the number of active, inactive, and abandoned wells, and the monthly pumping rates were obtained from the respective utility. The average monthly pumping plot (Figure 11) reveals a greater demand for water throughout the summer months of May to August, and an upward linear trend for water usage between 1960 and 2000, also seen by Criner and Parks (1976) and Hutson et al., (2004), with a slight decline and steady rates towards 2021, matching countywide values reported by Kenny et al. (2009) and Dieter et al. (2018).

The monthly pumping rates for individual wells in all MLGW and municipal well fields (Figure 1) were computed by evenly dividing the cumulative monthly pumping rates by the number of active producing wells in each well field each month (Villalpando-Vizcaino et al. 2021). For missing pumping records, the monthly rate for a particular year was computed using Equation 1 by Torres-Uribe et al. (2021).

$$\mathrm{MPR_i} = \mathrm{MPR_{i-1}} * \left(1 + \frac{\mathrm{ADP_i} - \mathrm{ADP_{i-1}}}{\mathrm{ADP_i}}\right) * \frac{\mathrm{AW_{i-1}}}{\mathrm{AW_i}} \quad (1)$$

Where, $\mathrm{MPR_i}$ is the monthly pumping rate for a missing month of a year, $\mathrm{MPR_{i-1}}$ is the monthly pumping rate of the same month in the previous year, $\mathrm{ADP_i}$ is the average daily withdrawal of a given year, ADP_{i-1} is the average daily withdrawal of the previous year, AW_i and AW_{i-1} are the number of active wells in a giver year and a previous year, respectively.

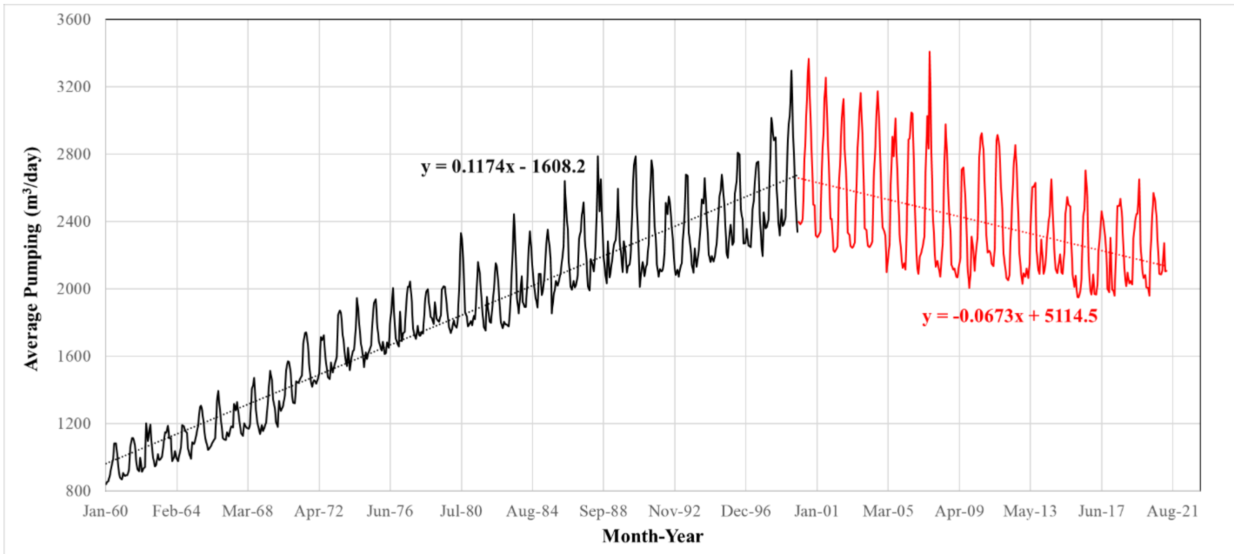

Figure 11. Plot of mean monthly pumping rate among 345 wells during the period 1960 to 2021. Black line indicates upward linear trend (1960-2000), and red line indicates downward trend (2000-2021).

Model calibration

The CAESER-II model was calibrated using automated Parameter ESTimation (PEST) (Doherty, 2015; Doherty et al., 2011; Doherty and Hunt, 2010) over the simulation period 1960-2021, to match simulated heads from observation wells and monitoring points. For comparative analysis and to account for heterogeneity, the CAESER-II model was calibrated using the same number of parameters (938 pilot points and 36 zones), observation wells, and monitoring points data from the CAESER-I model yet using more historical observed readings. The model was parameterized using pilot points (mathematical regularization) of varying density for parameters hydraulic conductivity and specific storage. Additionally, parameters such as riverbed conductance, specific yield and recharge in the unconfined portion of the Memphis aquifer were parameterized by zones (manual regularization). Following Villalpando-Vizcaino et al. (2021), a total of 74 observation wells for the shallow, Memphis, and Fort Pillow aquifers were used, as well as the monitoring points data were updated from historical water table/water level maps (Criner and Parks 1976; Graham 1982; Parks 1990; Parks and Carmichael 1990c; Kingsbury 1992, 1996; Konduro-Narsimha 2007; Schrader 2007; Ogletree 2017; Kingsbury 2018), in accordance with Hill and Tiedeman (2007).

Initial values of pilot points and zones were obtained from previous modeling efforts, and hydrogeologic reasonableness was considered during calibration process (Anderson et al. 2015). As pumping test data and breach Kv were available at some locations, Tikhonov regularization (preferred values) was used so that parameters should adhere to defined values (Anderson et al. 2015). Owing to the large number of pilot points and ill-posed inverse problem, Singular Value Decomposition (SVD) was used to reduce the number of parameters to the effective estimable components (Doherty and Hunt 2010).

Results and discussion

After transient calibration, the parameters approached values resulting in the smallest possible error. Figure 12 illustrates the distribution of calibrated pilot point values for hydraulic conductivity derived from the calibrated CAESER-II model. Most points fall within the range of published literature and generally accepted values. Due to the presence of gravel, the average horizontal hydraulic conductivity of the shallow aquifer is higher than that of the Memphis aquifer (19.6 m/day compared to 18.1 m/day). A similar phenomenon was observed in the CAESER-I model, which predicts average horizontal hydraulic conductivities of 20.9 and 18.4 m/day for the shallow and Memphis aquifers, respectively. The Fort Pillow aquifer had a lower mean horizontal hydraulic conductivity (9.8 m/day) than other aquifers due to the higher proportion of finer sediments (Criner and Parks 1976), and the CAESER-I model reports a similar value.

Conductivity values for the confining units UCCU and Flour Island are consistent with values for clay-based aquitards and match the order of magnitude predicted by the CAESER-I model. On the other hand, the breach horizontal conductivity has a wide range (Figure 12(b)) with an average value of 0.76 m/day, indicating that the vertical conductivity (Kv) would be 0.076 m/day, matching closely to the falling head test results of the soil analysis at 99s2.

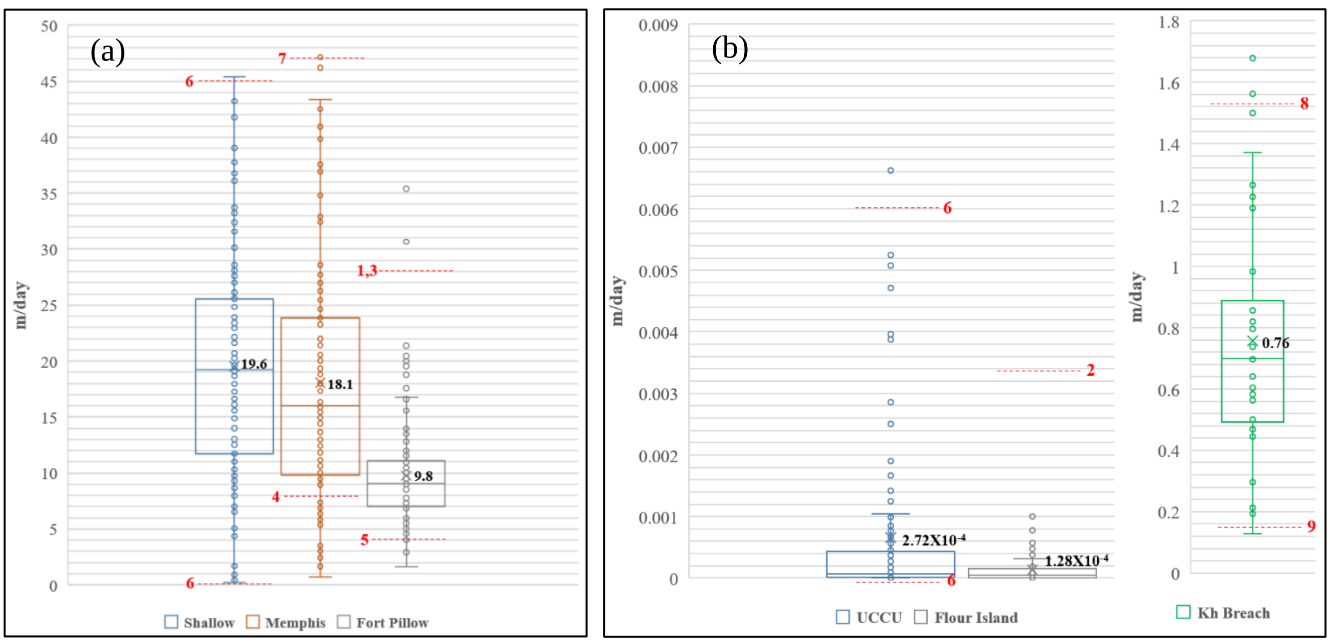

Figure 12. Calibrated hydraulic conductivity values at pilot points for (a) aquifers and (b) confining units. Published values are showing as red dashed lines with references: [1](Schneider and Cushing 1948), [2](Graham and Parks 1986), [3](Parks and Carmichael 1989), [4](Parks and Carmichael 1990b), [5](Carmichael 1997), [6](Robinson et al. 1997), [7](Gentry et al. 2006a), [8](Torres-Uribe et al. 2021) and [9]Larsen et al. (2013).

Calibrated, average specific storage values are 0.0018 m^{-1} for the UCCU, 0.0033 m^{-1} for the Memphis aquifer, which matches the order of magnitude of Sahagún-Covarrubias et al. (2022)

with an average of 0.0022 m^{-1} and 0.0018 m^{-1} for the Flour Island confining unit and Fort Pillow aquifer. These values fall within the ranges provided by Criner et al. (1964) and Parks and Carmichael (1989, 1990b). Riverbed conductance varied between 1.06 to 11.68 m/day, not changing much from Villalpando-Vizcaino et al. (2021) likely because the sensitivity scale of this parameter is low during calibration. Modeled recharge ranges between <1 cm/year to 9.3 cm/yr. Publish reports in the Shelby County reported recharge range of less than 1 cm/year to >10 cm/year (Clark and Hart 2009; Villalpando-Vizcaino et al. 2021).

Table 3 shows common calibration statistics for CAESER-I and CAESER-II for the shallow, Memphis and Fort Pillow aquifers. The modified model shows slight improvement over the original model within the time period 2005-2016. However, the RMSE for the Fort Pillow aquifer over the period 1960-2021 is large due to the lack of starting heads data in 1960, the absence of West Memphis pumping data, and a no-flow boundary that may not be able to support water for nearly 60 years of run time. Analysis of the water levels of all monitoring wells within the model revealed that the Memphis aquifer monitoring wells experienced the maximum of 68 m of water level change, greatest change among all the aquifers. Given the range of water levels in the model area and assuming a fraction of 5 percent, the permissible mean absolute residual (MAR) would be around 3.5 m. The CAESER-II model has MAR of 3.31 m for the entire model. In addition, the maximum simulated-to-observed head difference at a monitoring well (Sh:Q-059) was 7.2 m, and the average thickness of the Memphis aquifer is 210 m, so the error in head represents only 3.4% of the Memphis aquifer thickness.

Table 3. Mean measure of error (m) of all monitoring wells observed and simulated head values in Shallow, Memphis and Fort-Pillow aquifer.

`	**CAESER**-I (2005-2016)		**CAESER**-II (2005-2016)		**CAESER**-II (1960-2021)	
	MAR	**RMSE**	**MAR**	**RMSE**	**MAR**	**RMSE**
Entire model	1.57	2.03	1.53	2.01	3.31	4.15
Shallow	1.8	2.2	1.48	1.80	2.37	2.83
Memphis	1.4	1.8	1.42	1.94	3.19	3.94
Fort Pillow	1.8	2.3	1.75	2.25	4.12	5.13

Specific to the Sheahan well field, Torres-Uribe et al., (2021) compared the simulated and observed head in the Memphis aquifer using six observation wells as shown in Figure 7 (Sh:P-061, Sh:P-076, Sh:K-021, Sh:K-066, Sh:K-110 and Sh:K-122) resulting in a mean absolute residual (MAR) of 3.91 m, whereas the current CAESER-II model has a MAR equal to 3.70 m for the same observations wells and within the same time range 1960-2016.

Figure 13 depicts the hydrograph of simulated versus observed head time series of monitoring wells in the Sheahan well field, including one in the shallow aquifer (Sh: K-075), two in the Memphis aquifer (Sh:M-040 and Sh:K-021), and one in the Fort Pillow aquifer (Fa:R-001). All the monitoring wells used for hydrograph analysis are shown in Figure 3 and monitoring well (Sh:M-040) was reported by Villalpando-Vizcaino et al. (2021). The hydrograph shows comparable goodness-of-fit in terms of visualization; however, Figure 13(c) shows that higher error was found between 1975 and 2000 since the majority of municipal well fields had only a snapshot of data before 2000. It has been found that increasing the pumping rate between 1975 and 2000 by a factor of 1.5 or, 2 and setting the highest limit as maximum pump capacity reduces the measure of errors for the entire model. But altering the pumping rate by a factor of multiplication will generate a bias in the head calculation, and this increase cannot be justified.

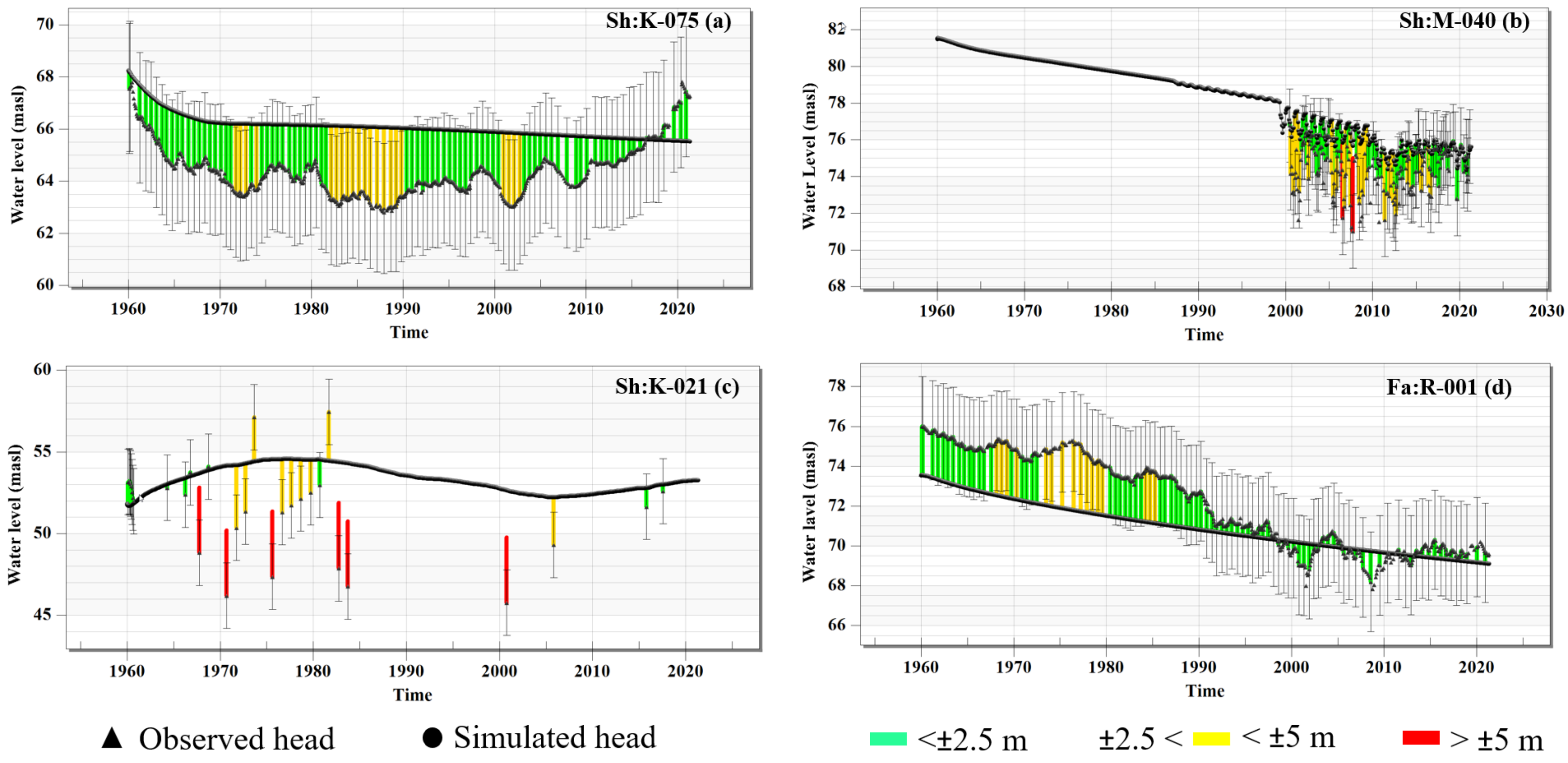

Figure 13. Hydrographs showing simulated and observed heads for monitoring well (a) Sh:K-075 (shallow aquifer), (b) Sh:M-040 (Memphis aquifer), (c) Sh:K-021 (Memphis aquifer), and (d) Fa:R-001 (Fort Pillow aquifer).Here, Sh:M-040 was also reported in CAESER-I model.

In addition, a sensitivity analysis was conducted to comprehend the uncertainty around the breach vertical hydraulic conductivity (Kv). By increasing the Kv for all breaches with a same value from 0.0002 m/day to 1.5 m/day, the root-mean-square error (RMSE) was determined for the Memphis aquifer observation wells. Figure 14 demonstrates that the Kv of breach(es) has a sensitive zone between 0.0015 and 0.1 m/day.

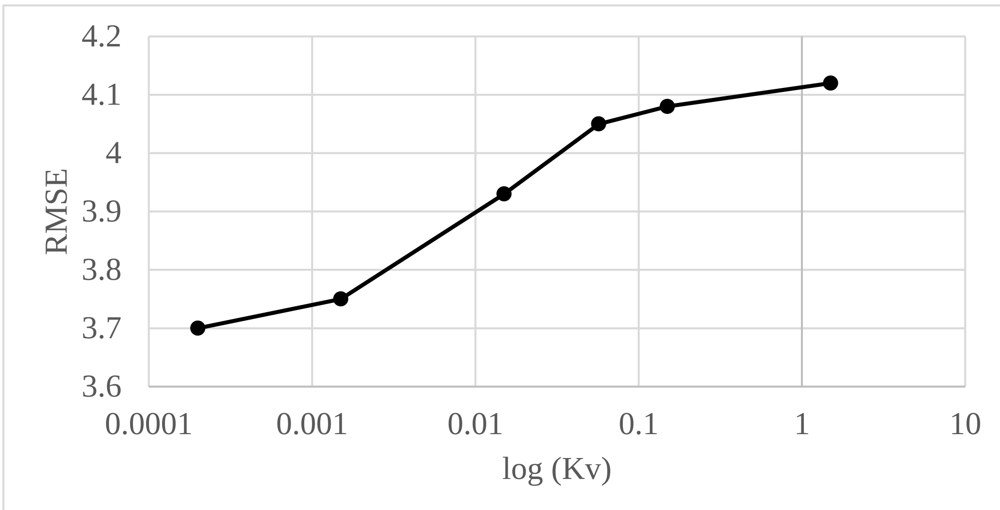

Figure 14. RMSE in Memphis monitoring wells with variations in breach vertical hydraulic conductivity (Kv)

Conclusions

The existing Shelby County groundwater flow model (CAESER-I) was updated and re-calibrated to simulate the groundwater flow dynamics within individual hydrogeologic system. Although the CAESER-II model has similar conceptualization of CAESER-I, the modified version improves upon on five different criteria, which include (1) extend the model from 1960 to 2021, (2) update the hydraulic parameters of the Memphis aquifer, (3) geometry modification of Parks (1990) breach at Sheahan well field, (4) characterize the hydraulic properties of an breach, (5) incorporate available historical pumping and river stage data. Following transient calibrations, the updated groundwater flow model showed improvement than the extended model by Torres-

Uribe et al. (2021) and the CASER-I model. Thus, CAESER-II model will be used for predictive simulations and may eventually be coupled with the flow model to simulate contaminant transport.

Aquitard breaches add significant local complexity to groundwater flow and play a dynamic role in modeling inter-aquifer exchange (Waldron et al. 2011) and contaminant transport, so better characterization of breaches could enhance modeling efforts. Again, breaches could lead to areas of local dewatering, resulting in the formation of dry cells that account for numerical error in the unconfined aquifer or UCCU layers. Therefore, implementing additional surface processes such as adjusting areal recharge, evapotranspiration, and tributary streams could alleviate the problem of dry cells and enhance the modeling of shallow unconfined aquifer or UCCU layers (Pierce, 2022). The spatial distribution of recharge could also be updated by incorporating zones based on land use and land cover map (Mensah et al. 2022).

In the future, certain modifications might be made to the model. For instance, the western part of the shallow aquifer is set by the Mississippi River, but the river could be attached with the Mississippi River Valley alluvial aquifer (west of the Mississippi River bluff) instead of shallow aquifer (east of the Mississippi River bluff). Also, the eastern part of Memphis aquifer is set as a constant head boundary based on only one monitoring well (Fa:R-002). Near this boundary is the Shaw well field, which has supplied water to communities in eastern Shelby County and has increased pumping in recent years (Moore 2021). As such, the eastern boundary should be reevaluated based on additional water level data near the boundary. In addition, in the CAESER-II model, heterogeneity for aquifer parameters at layer 3 was applied uniformly to layers 4-6, which represent the Memphis aquifer. Therefore, the vertical heterogeneity of the Memphis aquifer layers could be taken into account by incorporating distinct pilot point sets for layers 3-6.

Again, the spatial pattern of recharge could be updated by incorporating zones based on land use and land cover map (Mensah et al. 2022). Thus, the numerical model should continue to be refined and updated to accurately simulate flow by representing the complex geometry of geologic structures (Meyer et al. 2014).

Even if the hydraulic parameters for CAESER-II model are within the published range, the spatial distribution of parameters does not necessarily reflect the only true distribution of parameters (Doherty 2015). Like, Sahagún-Covarrubias et al. (2022) attempted to evaluate the hydraulic properties of the Memphis aquifer, but only measured parameters at five well fields which were used to constrain the model at those locations during calibration. There is a need for additional physical measures, such as aquifer testing and breach Kv, to restrict the model during calibration and to realize model input uncertainty. Thus, to know the most probable spatial distributed parameters it is necessary to identify a subset of equally calibrated models in terms of uncertainty analysis (Anderson et al. 2015; Doherty 2015). The calibrated groundwater flow model provides a management tool for the Shelby County and will aid in making appropriate management decisions within the range of uncertainty.

INVESTIGATION OF MODERN LEAKAGE

Introduction

Assessing aquifer vulnerability to contamination or water quality loss is essential for protecting and managing groundwater resources, particularly in areas where groundwater is the sole source of potable water (Almasri 2008; Fannakh and Farsang 2022). This situation can be exacerbated in urban and industrialized areas since the groundwater may be affected by pollution caused by anthropogenic sources that were or are being disposed of improperly (Ponzini et al. 1989). Also, to fulfill the increased demand for water in urban areas, excessive groundwater pumping can result in increased vertical downward gradients and deep infiltration of urban runoff or leachate into water supply aquifers (Larsen et al. 2013, 2016). For this reason, confined aquifer systems separated by aquitards are generally preferred for water supply purposes because aquitards may prevent contamination of underlying aquifers and limit recharge from surface sources of lesser quality (Cherry et al. 2006; Hart et al. 2006). The water supply aquifer may be semi-confined in some areas, where pumping locally increases downward hydrologic gradients, causing leakage from the upper shallow aquifer to the underlying water supply aquifer.

Memphis and neighboring municipalities (Figure 1) rely heavily on groundwater from the confined to partially confined Memphis aquifer (Criner and Parks 1976; Parks 1990; Dieter et al. 2018). The Memphis aquifer is mostly confined by an aquitard unit comprised of varying quantities of low-conductivity materials such as silts and clays, termed the upper Claiborne confining unit (UCCU) (Graham and Parks 1986; Parks 1990).

In previous studies, it was initially assumed that throughout the Memphis area, the UCCU confined and protected the Memphis aquifer with an average of 43 m of clay except in the outcrop area in the eastern part of Shelby County (Figure 1) (Cushing et al. 1964; Larsen et al. 2003; Gentry et al. 2006b). Most recently, studies suggest that there are “breaches” where the clay unit is thin (< 3 m thick) or absent in some areas of the UCCU (Figure 1) (Parks 1990; Parks et al. 1995; Gentry et al. 2006a, b; Waldron et al. 2009; Larsen et al. 2013; Jazaei et al. 2019). These breaches create preferential pathways between the shallow and Memphis aquifers, whereby an overall downward vertical gradient created by extensive pumping, induces leakage of degraded water quality from the shallow aquifer into the underlying Memphis aquifer (Graham and Parks 1986; Parks 1990; Larsen et al. 2003, 2016; Waldron et al. 2009, 2011; Carmichael et al. 2018). Previously published age-dating results in Shelby County indicate the presence of as much as 30 percent modern water (<60 years) produced from Memphis aquifer municipal wells near some of these breaches, with age ranges of 20 to 45 years (Larsen et al. 2013, 2016). Though challenging, a better understanding of the magnitude and recharge pathway of inter-aquifer flow through breaches is required for assessing the vulnerability and sustainability of a well field (Medici et al. 2016).

Identifying and characterizing aquitard breaches requires costly detailed subsurface geological investigations (Gentry et al. 2006a; Waldron et al. 2009; Jazaei et al. 2019). Several studies have identified aquitard breaches indirectly by evaluating anomalous water-table depressions, stream loss estimation, borehole log stratigraphy showing absence or thinning of the UCCU, geophysical methods, and geochemical investigations (Parks 1990; Bradley 1991; Larsen et al. 2003; Gentry et al. 2006a; Waldron et al. 2009). These methodologies have inherent limitations and are also constraint by resources and spatial effectiveness; hence, several studies in Shelby County indicate that numerical modeling investigations are a valuable tool for defining recharge pathways and quantifying downward leakage through the UCCU (Brahana and Broshears 2001; Jazaei et al. 2019; Torres-Uribe et al. 2021; Villalpando-Vizcaino et al. 2021).

Jazaei et al. (2019) used a numerical model to identify possible leaky aquitard zones in the UCCU near three well fields, Allen, Davis, and Palmer, which are operated by MLGW, the largest utility company for Memphis and unincorporated Shelby County. The study identified five suspected breach zones using pilot-point calibration, velocities, flow budget, and particle tracking. Of these five leaky zones, three (zones 1, 2, and 4) were validated by previous studies (Parks and Carmichael 1990a; Carmichael et al. 2018).

Villalpando-Vizcaino et al. (2021) developed a multi-layered, 3D groundwater model (referred to as CAESER-I and depicted in Figure 1) to assess inter-aquifer exchange between the water-table (shallow), Memphis, and Fort Pillow aquifers as separated by their confining units. Total leakage from the UCCU into the Memphis aquifer was estimated at 61.1 m^3/min, accounting for 10.4% of the total Memphis aquifer inflows during August 2016, with higher leakage observed at breach locations. However, the upper 60 m of the Memphis aquifer received leakage contributions from the UCCU leakage of almost 30%.

Torres-Uribe et al. (2021) extended the groundwater model developed by Villalpando-Vizcaino et al. (2021) backward in time to January 1960 to assess the spatial configuration of breaches near MLGW’s Sheahan well field in south-central Shelby County. By comparing simulated parameters against published age-dating and geochemistry data, they suggested the presence of a large and spatially extensive paleochannel formed by erosional processes and filled with sand and gravel of the shallow aquifer, overlying thinned UCCU. In addition, Larsen et al. (2013)

suggested that shallow groundwater from Nonconnah Creek migrates along the paleovalley and potentially recharges the upper Memphis aquifer through the breach locations.

As part of Torres-Uribe et al. (2021) modeling efforts, particle tracking (MODPATH) was used to simulate the flow paths of modern water into the Memphis aquifer using the extended CAESER-I model. An issue with particle tracking is that it only considers the advective transport of particles (Pollock 2016), whereas flow paths could be affected by dispersive movement (Bethke and Johnson 2008). Therefore, this study considers the movement of modern water using the advection-dispersion equation (Dagan and Nguyen 1989) while computing the mean age and mixing percentage.

Additionally, the combined application of tracers and geochemical modeling has been used throughout the years to estimate and assess the modern water leakage in the Sheahan well field (Larsen et al. 2003, 2016; Gentry et al. 2006b; Kingsbury et al. 2017). Age-dating tracers (^{3}H and ^{3}He) can identify production wells containing modern water and yield mean ages, which are evaluated against hydrogeologic data to identify potential leakage sources and pathways. Also, environmental tracers yield mixing percentages of modern water using lumped parameter modeling (LPM) that considers simplified aquifer settings and groundwater flow dynamics (Jurgens et al. 2012). On the other hand, geochemical modeling of water chemistry using the United States Geological Survey (USGS) PHREEQCi program has been used in several well fields in Shelby County, including Sheahan, to estimate the mixing percentage of shallow groundwater with Memphis aquifer water in the vicinity of production wells (Larsen et al. 2003, 2013; Koban et al. 2011).

This research presents a case study of integrated hydrostratigraphic analysis, numerical modeling, hydrologic tracers, and geochemical modeling to evaluate the local leakage process and potential migration pathways of modern water from the shallow aquifer to the underlying water supply aquifer. This study presents a comprehensive analysis of the Sheahan well field production wells, using groundwater age and geochemical signatures to substantiate the presence of additional breaches within the UCCU beyond those previously published. This multifaceted approach refines the likelihood of a large paleochannel structure identified by Torres-Uribe et al. (2021) that could provide preferential flow horizontally within the water-table aquifer, which then migrates downward through the UCCU into the Memphis aquifer.

Regional Hydrogeology

Memphis, Tennessee, is located within the Mississippi embayment, a trough-shaped aquifer system which is filled with approximately one kilometer of unconsolidated and semi-consolidated sediments (Graham and Parks 1986; Brahana and Broshears 2001; Waldron et al. 2011). As shown in Figure 2, the subsurface is underlain by three water-bearing sand aquifers: the shallow unconfined aquifer (also referred to as the water-table aquifer), the Memphis aquifer, and the Fort Pillow aquifer, each of which is separated by aquitard unit (Brahana and Broshears 2001; Clark and Hart 2009).

The shallow aquifer consists of fluvial-terrace deposits of Pleistocene and Pliocene age and alluvial deposits of Holocene and Pleistocene age, which are overlain by Pleistocene loess and underlain by Eocene upper Claiborne confining unit (Parks 1990). The shallow aquifer is composed mostly of sand and gravel with horizontal hydraulic conductivity ranging from 1.5 to 45 m/day (Graham and Parks 1986). This aquifer is locally contaminated due to the absence of an overlying aquitard, so groundwater from the Memphis and Fort Pillow aquifers serves as the primary water source for Memphis and its surrounding communities (Graham and Parks 1986).

The UCCU unit mostly separates the Memphis aquifer from the overlying shallow aquifer, except for the areas of local discontinuities known as breaches and along the eastern border of Shelby County, where the UCCU unit is absent (Parks 1990) (Figure 1). The UCCU unit can be subdivided into the Cockfield and Cook Mountain formations (Graham and Parks 1986). In general, the Cockfield Formation is composed of clay and silt in the upper portion and fine sand in the lower portion, with highly variable thickness (Parks and Carmichael 1990a). The Cook Mountain Formation consists predominantly of clay but contains variable quantities of sand in localized areas (Parks and Carmichael 1990b) and is the main confining clay for the Memphis aquifer (Carmichael et al. 2018). This unit ranges in thickness from 0 to 110 meters (Graham and Parks 1986), and vertical hydraulic conductivity ranges from 1.5×10^{-6} to 3.0×10^{-4} m/day (Robinson et al. 1997). Though there is uncertainty in breach vertical conductivity, several studies have identified a range between 1×10^{-4} to 0.1524 m/day (Gentry et al. 2006a; Torres-Uribe et al. 2021; Villalpando-Vizcaino et al. 2021; Paul 2022).

The Memphis aquifer is composed of fine to coarse sand with clay lenses and becomes unconfined in east-southeast Shelby County as the Memphis aquifer is composed of the Memphis Sand of the Claiborne Group (Parks 1990). The Memphis Sand ranges from 150 to 270 m thick, and horizontal hydraulic conductivity varies between 2.9 to 47 m/day (Parks and Carmichael 1990b; Sahagún-Covarrubias et al. 2022). The Memphis aquifer is separated from the deeper Fort Pillow aquifer by the Flour Island confining unit, which consists primarily of clay and varies in thickness from 50 to 95 meters (Graham and Parks 1986). The Fort Pillow aquifer consists mainly of sand with an average thickness of 60 m and overlies the Old Breastworks confining unit, which is primarily clay (Parks and Carmichael 1989).

Sheahan well field

The Sheahan well field (Figure 15) has 24 production wells and a pumping station with a treatment capacity of 35 x 10^6 liters per day and has been operational since 1932 (Larsen et al. 2003). Evidence of vertical leakage through breaches in the UCCU unit has been characterized by numerous geological, environmental tracers, and geochemical studies (Graham and Parks 1986; Parks 1990; Larsen et al. 2003, 2013, 2016; Gentry et al. 2006a; Murphy 2017). Using borehole and water-level data, Parks (1990) showed a potential breach location at the western side of the Sheahan well field. Later studies (Larsen et al. 2003, 2016; Gentry et al. 2006a; Ivey et al. 2008) have attempted to evaluate the presence and extent of additional breaches than those published by Parks (1990) and the extent of modern water recharging the Memphis aquifer. Most recently, Torres-Uribe et al. (2021) suggested the presence of a large and spatially extensive paleochannel atop the UCCU. Also, three breaches (near 99s2, FCCMW19/FCCMW20 and 78B) were identified from drilling results and using a contour map of the aggregate thickness of confining clay within UCCU as shown in Figure 16. Breaches near the central and western part of well field were validated by additional drilling and thus refine the paleochannel configuration defined by Park (1990). Recent modifications of the CAESER-II model (Figure 1(c)) with these three breach locations provide a more accurate representation of groundwater flow dynamics between shallow and Memphis aquifers at Sheahan well field.

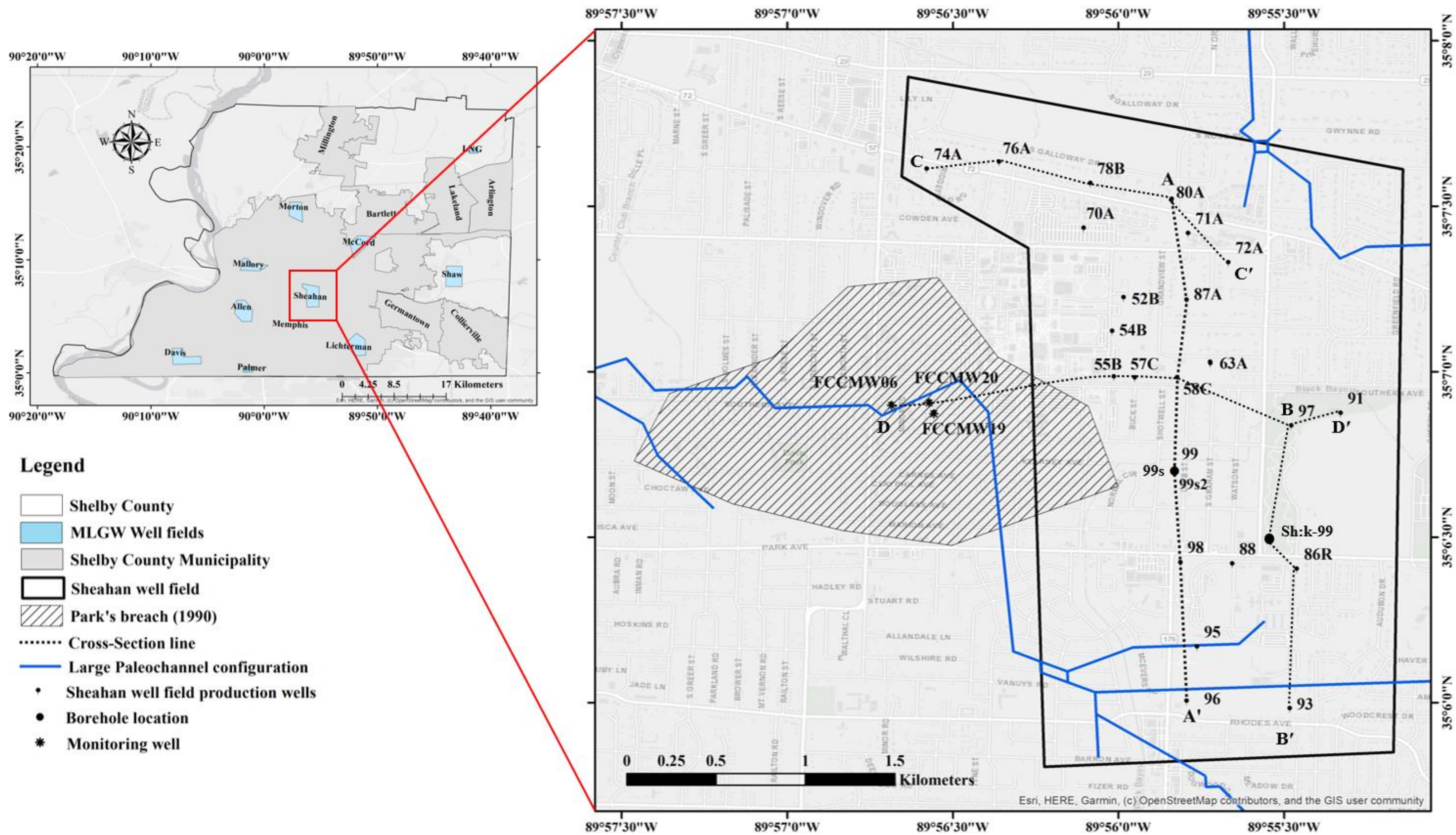

Figure 15. Layout of MLGW's Sheahan well field and municipalities in Shelby County. Also shown are borehole locations, Parks (1990) breach, the large paleochannel formation defined by Torres-Uribe et al. (2021), and cross-section lines at the Sheahan well field.

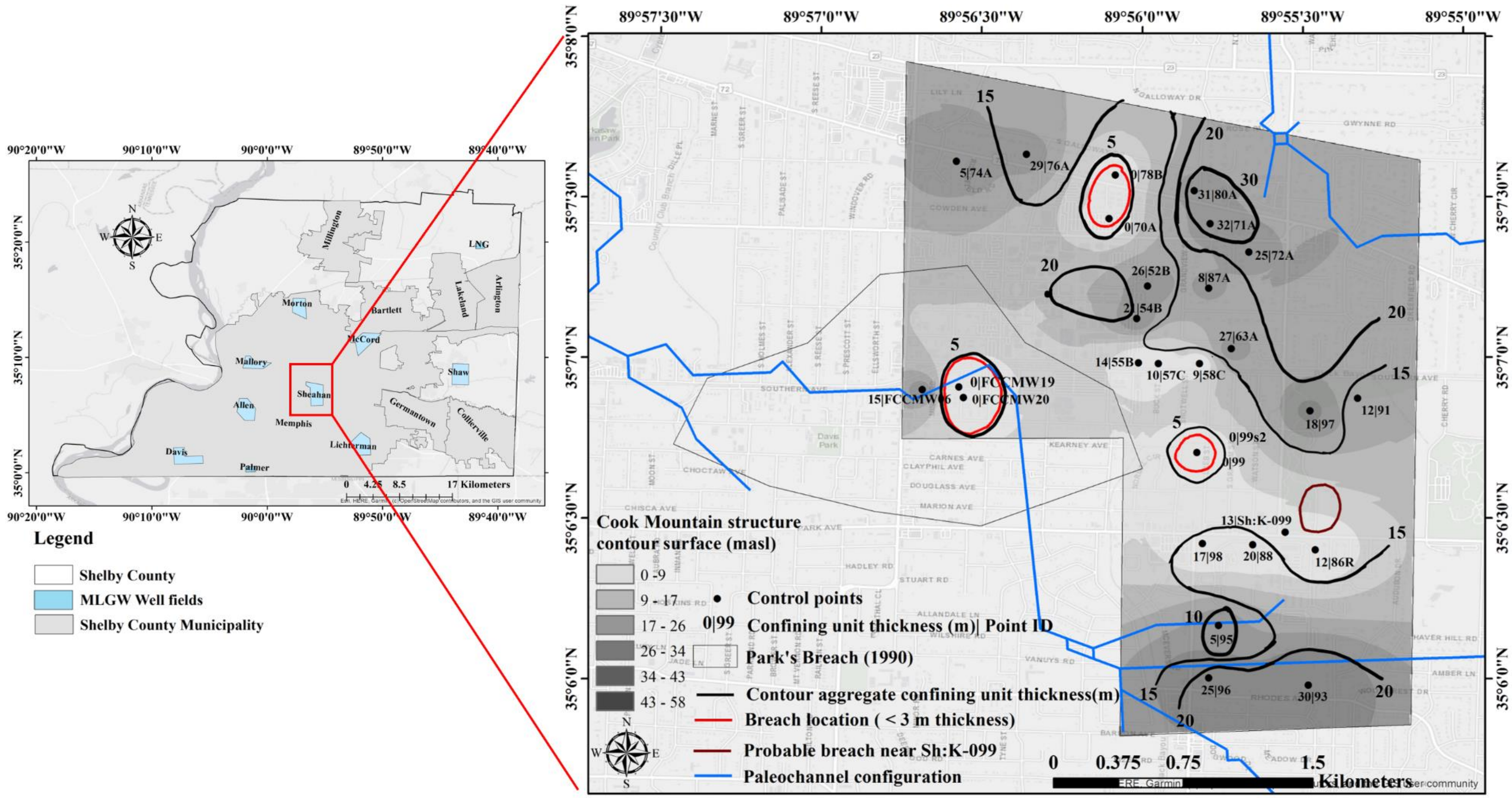

Figure 16. Contour map illustrating the aggregate thickness of confining clay within the UCCU. Thinned areas represent potential Cockfield paleochannels incised into and, in some areas, completely eroding the Cook Mountain Formation.

Therefore, the general recharge mechanism is that water from Nonconnah Creek travels along the paleochannel within the shallow aquifer toward the Sheahan well field before leaking into the Memphis aquifer through the breach locations, similar to that suggested by Larsen et al. (2013).

Methods

Hydrogeologic Cross Sections

The cross-sections were constructed from geophysical, driller and geologist logs to evaluate local subsurface geology. The hydrogeologic units: loess, shallow aquifer (fluvial-terrace deposits), UCCU (Cockfield and Cook Mountain formations) and Memphis aquifer (Memphis Sand) were identified by characteristic changes in the natural gamma and electrical resistivity logs. The interpretation and designation of the lithological and hydrostratigraphic units are based on the correlation of core samples to geophysical data (Carmichael et al. 2018; Larsen et al. 2022) and field-based geologic studies in the Memphis area (Vanderlip et al. 2021).

Groundwater Sampling

A total of eight production wells (57C, 58C, 63A, 97, 86R, 54B, 87A, and 96) screened at different depths in the Memphis aquifer, and one water-table aquifer monitoring well (99s) screened in the Cockfield Formation in the Sheahan well field were sampled in the summer of 2020 (Figure 15). To avoid degassing and ensure a representative sample, production wells were pumped for more than 12 hours at a discharge pressure greater than 200 kPa prior to sampling (Larsen et al. 2003, 2016; Gentry et al. 2006a). Monitoring well (99s) was redeveloped before sampling to remove any accumulated sediment and biological film from the screen (Yeskis and

Zavala 2002). Following re-development, three-borehole volumes of water were purged from the monitoring well to ensure a representative aquifer sample. A Grundfos submersible pump with a flow rate of 0.341 m^3/h was used to redevelop and collect samples maintaining low-flow conditions, similar to Larsen et al. (2013).

Field parameters, including temperature, pH, dissolved oxygen (DO), specific conductivity (SC), oxidation-reduction potential (ORP) and turbidity, were monitored and recorded with calibrated In-Situ AquaTroll 500 Multi-Parameter Water Quality Sonde. Additional field measurements to verify the AquaTroll data were made for pH (using Thermo Fisher Scientific Orion Star A324 pH/Ion Selective Electrode), DO (using YSI model 95 Handheld Dissolved Oxygen Meter), SC (using Oakton Cond 6+ Handheld Conductivity Meter) and Turbidity (using Thermo Fisher Orion AQ3010 Turbidity Meter). Also, total alkalinity was measured using a Hach Total Alkalinity Method 8203 Titration Kit with 0.16 M sulfuric acid in the field.

Once field parameters stabilized and turbidity was less than 2 NTU, water samples were collected for dissolved metals and anions, semi-volatile organic compounds (SVOCs), and volatile organic compounds (VOCs) for analysis at Waypoint Analytical Laboratory in Memphis, Tennessee, using EPA drinking water methods (6020B, 7470A, 8260B, 8270D, and 9056A). The water quality samples for the Waypoint Analytical Laboratories were kept in an ice-filled cooler and delivered the same day for chemical analysis.

Samples for ^{3}H were collected in 1-liter amber glass bottles, and bottle caps were tightly sealed with tape to prevent the exchange of atmospheric vapor. These bottles were placed in a refrigerator at 4℃ before shipping to the Noble Gas Laboratory at the University of Utah. For each production well, a gas diffusion sampler comprised of a copper tube with a semi-permeable membrane was used to measure the noble gases (Gardner and Solomon 2009). The diffusion sampler was deployed in a flow-through cell and allowed to equilibrate with the flow of production well water for about 24 hours at a constant back pressure of 275 to 289 kPa (Larsen et al. 2003). After retrieving and sealing the diffusion samplers, a calibrated Pentair Point Four Tracker Portable TGP meter was used to measure the total gas and barometric pressure in the flow-through cell. For the monitoring well, however, the diffusion sampler was affixed to a string with additional weight and placed in the screened interval for one week before retrieving and sealing. The total gas pressure and barometric pressure were measured during water quality sampling.

The tritium samples and diffusion samplers were sent to the University of Utah's Dissolved Gas Lab for analysis. Tritium was analyzed using the helium in-growth method with a detection limit of 0.05 TU (Solomon and Cook 2000). Dissolved gases were analyzed using the method of Bayer et al. (1989). Reactive gases were removed using a SAES getter (degassing device), and heavy noble gases were sorbed onto charcoal at –180˚C for Ar, Kr, and Xe, and at –236˚C for Ne. Helium and other noble gas isotopes were then measured on a MAP 215-50 mass spectrometer to a precision of approximately ±0.5%. Noble gas composition was used to determine the recharge temperature by applying a modified form of the closed-equilibrium model developed by Aeschbach-Hertig et al. (1999). Tritiogenic helium was calculated using Ne to correct for the excess atmospheric gas entrained during water percolation through the vadose zone and applied along with ^{3}H data in the groundwater age equation of Solomon and Cook (2000).

Data analysis

The water chemistry of the production and monitoring wells was analyzed to determine a linear trend/mixing relationship between the Memphis aquifer and the overlying shallow (water-table) aquifer, similar to Larsen et al. (2003, 2013). A piper diagram was created to characterize the water types in the Sheahan well field. Cross-plots were used to identify end members for water-table and Memphis aquifer water compositions.

Inverse Geochemical Modeling

Inverse geochemical modeling was performed using PHREEQCi version 3 software for simulating chemical reactions and transport processes (Parkhurst and Appelo 2013). PHREEQCi estimates mineral phases and probable mixing ratios considering end member compositions and aquifer mineral reactions (Larsen et al. 2003, 2013). The feasibility of the inverse modeling results was evaluated using the mix command in PHREEQCi considering geochemically reasonable mineral reactions. Several well field studies in Shelby County, Tennessee, have utilized this method to predict the mineral reactions and mixing percentage of modern water (Larsen et al. 2003, 2013; Gentry et al. 2006a; Koban et al. 2011). The modeled 2020 data for Sheahan well field were compared to the previous model by Larsen et al. (2016) to evaluate consistency and any potential temporal trend.

Lumped Parameter Modeling

Lumped parameter modeling (LPM) was performed with TracerLPM by parametrizing the simplified aquifer geometry and groundwater flow configurations that account for dispersion or mixing within the well bore (Jurgens et al. 2012). TracerLPM requires an appropriate LPM model that best fits the recharge condition based on the conceptualization of the physical system. The suitable LPM model was inversely fitted with the output tracer concentrations to the measured tracer concentrations by varying the mean age and other model parameters until the relative error was minimized. Models of exponential piston flow and dispersion are suitable for long-screened public supply wells (Eberts et al. 2012; Larsen et al. 2016). Binary mixing models can characterize two-component mixtures, which is a common occurrence in Sheahan well field, where superficial groundwater has infiltrated into the deep Memphis aquifer (Larsen et al. 2003; Ivey et al. 2008).

Solute Transport Modeling

To simulate shallow groundwater and Memphis aquifer water mixing, MT3DMS was used, a solute transport package based on the advection-dispersion equation (Zheng 1992). The CAESER-II numerical model was used to evaluate groundwater flow conditions for the solute transport model for the Sheahan well field. CAESER-II is an updated multi-layered model based on Villalpando-Vizcaino et al. (2021) (i.e., CAESER-I) that simulates the inter-aquifer water exchange from 1960 to 2021 in the Shelby County area between all three principal aquifers: shallow, Memphis, and Fort Pillow, and the two confining units, the UCCU and Flour Island. The CAESER-II model consists of eight layers, with Layer-1 representing the shallow aquifer, Layer-2 being the UCCU with aquitard breaches, Layers 3 to 6 representing the Memphis aquifer, Layer 7 representing the Flour Island and Layer-8 being the Fort Pillow aquifer. The

CAESER-II model was developed using the United States Geological Survey (USGS) MODFLOW-NWT program with a cell size of 250 m by 250 m.

Unlike the groundwater-flow model (CAESER-II), which includes all the municipal well fields in Shelby County, the solute transport model focused on the Sheahan well field. The contaminants migrate through the hydrogeologic strata primarily due to groundwater flow, but mechanical dispersion, molecular diffusion, and retardation also play a role. However, this study did not simulate molecular diffusion and retardation processes due to a lack of data for the aquifer media.

The transport model was calibrated to observe contaminant concentration by adjusting the longitudinal dispersivity. The source concentration was defined based on the historical data from the monitoring well at the source location. The primary potential contaminant source is the Former Custom Cleaners (FCC) site west of the Sheahan well field (Figure 16). A recent investigation by the Tennessee Department of Environment and Conservation (TDEC) revealed that perchloroethylene (PCE) was released from approximately 1950 to the mid-1990s during the dry-cleaning operation (Versar Inc. 2018). The remedial investigation report (EPA ID TN000402275) of this FCC site reported that PCE concentration at an onsite monitoring well (FCCMW19) was 0.14 mg/L in 2015 (Versar Inc. 2018). So, the initial concentration of PCE was set as 0.14 mg/L as a constant source from FCCMW19 (Figure 15).

Moreover, the scale-dependent longitudinal dispersivity was assigned an arbitrary value, which was then varied between 0.5 to 50 m. Longitudinal dispersivity of 15 m best fits existing data for PCE concentrations provided by the utility. In addition, the empirical equation to determine longitudinal dispersivity in unconsolidated media is given by equation 1 (Schulze-Makuch 2005). The nearest distance between the known contaminant site (FCC) and the production well (55B) is 750 m, so Equation 1 yields a longitudinal dispersity of 18 m. Also, Avon and Bredehoeft (1989) reported longitudinal dispersity for heterogeneous sediments is 15.2 m. Therefore, the longitudinal dispersivity of 15 m is reasonably justified, and the transverse horizontal and vertical dispersivities were kept at one-tenth and one-hundredth of the longitudinal dispersivity, respectively (Zheng and Bennett 1955).

$$\alpha_L = 0.085 * L^{0.81} \qquad (1)$$

Where, α_L is the longitudinal dispersivity, and L is the flow distance (m)

After calibrating the transport model, it was run to determine the mean age and mixing percentage at each sampled production well location. For this purpose, all breach locations were defined as contaminant sources, with the contaminant being modern water flowing from the shallow aquifer to the Memphis aquifer.

To calculate the mean groundwater age at a sampling location, modern water movement was modeled as multiple contaminant species, where each species entered the aquifer continuously within a specific timestamp (i.e., one year, for this case) following each other (Aghashahi 2023). Thus, 62 species were used to simulate the transient flow condition, and the mean age was calculated using Equations 2 and 3 (Aghashahi 2023).

$$P_{t_i}^{p} = \frac{C_{t_i}^{f}}{\int_0^T C_{t_i}^{f} dt}, \qquad i = 1, 2, \dots T \qquad (2)$$

$$\overline{A^p} = \int_0^T t_i P_{t_i}^p dt \qquad (3)$$

Where, C^f_t is flux concentration at each timestamp, ($P_t^p [\frac{1}{t}]$) is time probability at well location and $\overline{A^p}$ is the mean age.

On the other hand, to obtain the mixing percentage of the modern water in the Memphis aquifer water, we assigned constant head to cells representing breaches with an initial concentration of 100 mg/L and other cells were assigned an initial concentration of 0 mg/L (Lautz and Siegel 2006). Then, the concentration of solute at a well screen is defined by the mixing percentage at that location.

Results

Hydrogeologic Cross-Sections

The locations of the cross-sections are shown in Figure 15 with the cross-section drawings provided in Figure 10 and Appendix-A (Figures A1-A3). The thickness of the loess ranges from approximately 3.5 m to 11 m except at cross-sections C-C′, where no data exists up to 60 m above mean sea level (AMSL) at 78B. Beneath the loess, the fluvial-terrace deposits (shallow aquifer) extend to depths ranging from approximately 55 to 70 m-AMSL. A fine sand unit with sand/clay alteration, interpreted as the Eocene Cockfield Formation, typically extends to a depth of around 40 m-AMSL. The Eocene Cook Mountain Formation consists primarily of clay and ranges from about 0 to 31 m in thickness.

The Cockfield Formation is deeply incised through the Cook Mountain Formation and into the Eocene Memphis Sand at borehole 99s2 (cross-section A-A′). The absence of identifiable Cook Mountain Formation and forms in boreholes 58C and 98 suggests incision through the Cook Mountain Formation extends north and south of borehole 99s2, forming a broad paleochannel feature (Hasan et al. 2022). Similarly, at borehole 78B, the Cockfield Formation is incised into the Memphis Sand, suggesting another paleochannel exists at this site (cross-section C-C′). Additionally, cross-section D-D′ indicates that the Cook Mountain Formation is absent downgradient and east of boreholes FCCMW06, where recently installed monitoring wells (FCCMW19 and FCCMW20) verified the absence of clay in the UCCU (HydroGeoLogic Inc. 2022).

Water Quality and Chemistry

Water quality parameters monitored during the 2020 sampling event are summarized in Table 4. Temperature for Memphis aquifer wells ranged from 18.4 to 20℃. For comparison, the shallow groundwater in well, 99s (Figure 15), was 22.4℃ at the same time of production well sampling. pH varied from 6.04 to 6.62, with pH generally increasing with the depth of screen in the Memphis aquifer. Other parameter ranges include ORP from 25.2 to 204.2, conductivity from 0.099 to 0.153 mS/cm and DO from 1.05 to 1.37 mg/L, where DO decreases with the depth of the screened interval. DO at 99s was recorded as 4.0 mg/L in 2020.

Table 4. Field and chemical data from water sampling, Sheahan well field, 2020.

Well ID	**Sample date**	**Top of screen bgs (m)**	**Temperature (°C)**	**Specific conductance (mS/cm)**	**pH**	**ORP (mV)**	**Eh (mV)**	**Alkalinity (mg/L HCO_3)**	**DO (mg/L)**	**F^- (mg/L)**	**Cl^- (mg/L)**	**NO_3^- (mg/L)**
99s	7/27/2020	41	22.4	0.140	6.04	203	445	40.0	5.18	<0.125	9.12	3.53
87A	7/20/2020	95	20	0.153	6.1	162	406	61	1.21	<0.125	8.05	0.15
063A	7/13/2020	96	19.6	0.138	6.06	126	371	47.8	1.37	<0.125	6.88	<0.100
057C	7/13/2020	112	18.5	0.124	6.13	138	383	49.0	1.34	<0.125	4.43	<0.100
54B	7/20/2020	113	19.5	0.151	6.13	144	389	34.4	1.22	<0.125	7.88	0.188
54B (duplicate)	7/20/2020	113	na	Na	na	na	na	Na	na	<0.125	7.81	0.211
058C	7/13/2020	117	18.7	0.121	6.19	204	449	53	1.15	<0.125	4.48	<0.100
86R	7/15/2020	130	19.2	0.146	6.26	96.8	341	54.2	1.12	<0.125	5.5	<0.100
97	7/15/2020	144	18.4	0.099	6.23	151	397	45.1	1.29	<0.125	3.59	0.149
96	7/30/2020	211	19.8	0.130	6.62	25.2	269	59.6	1.05	<0.125	1.33	<0.100

Well ID	**SO_4^{2-} (mg/L)**	**Fe (mg/L)**	**Na (mg/L)**	**K (mg/L)**	**Ca (mg/L)**	**Mg (mg/L)**	**Turbidity (NTU)**	**As (µg/L)**	**Ba (µg/L)**	**Br (µg/L)**	**Hg (µg/L)**
99s	2.32	<0.100	15.8	0.303	5.32	2.83	na	<1.00	15.7	0.253	<0.0002
87A	12.3	0.62	12.6	0.832	8.02	3.55	na	<1.00	42.2	<0.200	<0.0002
063A	12.1	0.62	12	0.851	8.12	3.34	0.3	<1.00	32	<0.200	<0.0002
057C	6.77	<0.100	9.47	0.674	8.58	3.66	0.4	<1.00	24.9	<0.200	<0.0002
54B	13.7	0.48	12.4	0.715	9.06	3.88	na	<1.00	35.2	<0.200	<0.0002
54B (duplicate)	13.6	0.36	12.9	0.727	9.31	3.95	na	<1.00	35.5	<0.200	0.001
058C	7.01	0.23	9.05	0.687	8.44	3.58	0.2	<1.00	27.7	<0.200	<0.0002
86R	10.5	0.46	9.19	0.638	10.5	4.84	na	<1.00	34.4	<0.200	<0.0002
97	4.45	0.28	8.08	0.622	7.27	3.27	na	<1.00	26.5	<0.200	<0.0002
96	3.09	0.56	4.58	0.791	12.2	4.66	na	<1.00	19.5	<0.200	<0.0002

bgs = below ground surface, na = not available, <# below detection limit

Concentrations of Na^+, Cl^- and SO_4^{2-} decrease with depth, whereas other solute concentrations display variable trends with depth (Table 4), except for production well, 54B. Higher Na^+, Cl^-, NO_3^-, SO_4^{2-}, Fe and specific conductance were detected in the water at the production well 54B compared to other production wells with a similar screen depth. The chemistry of the shallow groundwater in the observation well, 99s, differs from that of the Memphis aquifer and has higher Na^+, Cl^- and NO_3^-. No volatile organic compounds (VOCs) and semi-volatile organic compounds (SVOCs) were detected, commonly found in pesticides and industrial solvents.

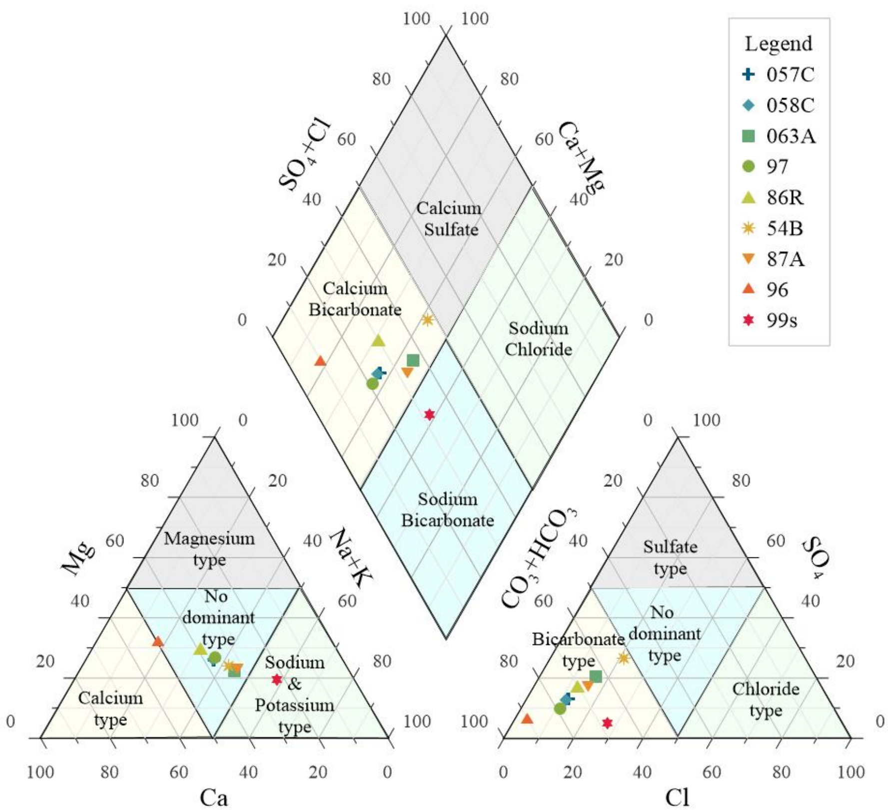

Figure 17. Piper diagram showing hydrochemical water types for Sheahan well field sampled during summer 2020.

Figure 17 illustrates the general hydrochemical composition of shallow groundwater and Memphis aquifer waters, which varies from no dominant to cation-HCO_3 type, similar to that observed by Larsen et al. (2003, 2013). Also, the water composition has not varied greatly in MLGW wells 86R, 87A, 57C, 63A, 54B, 096 and 99s from the sampling events of 1999 to 2020 (Figure A4, Appendix-A). Again, Figure 17 shows that Memphis aquifer water follows a linear trend in cation and anion concentration, and deep well 96 has elevated Ca^{2+} and HCO_3^- concentrations relative to other Memphis aquifer wells.

A cross-plot of two chemically conservative ions (sodium and chloride) is depicted in Figure 18. A linear mixture trend exists for all production wells and the shallow groundwater well (99s), and none follow the halite equilibrium line. The plot also shows 99s has higher amounts of sodium and chloride than the Memphis aquifer wells. Other cross-plots (Figure A5, Appendix-A) of alkalinity versus calcium and magnesium versus calcium illustrate a linear trend between shallow groundwater and Memphis aquifer water. For a few production wells, the cross-plot (Figure A5(a), Appendix-A) is aligned with the dolomite equilibrium line, but dolomite dissolution is not significant.

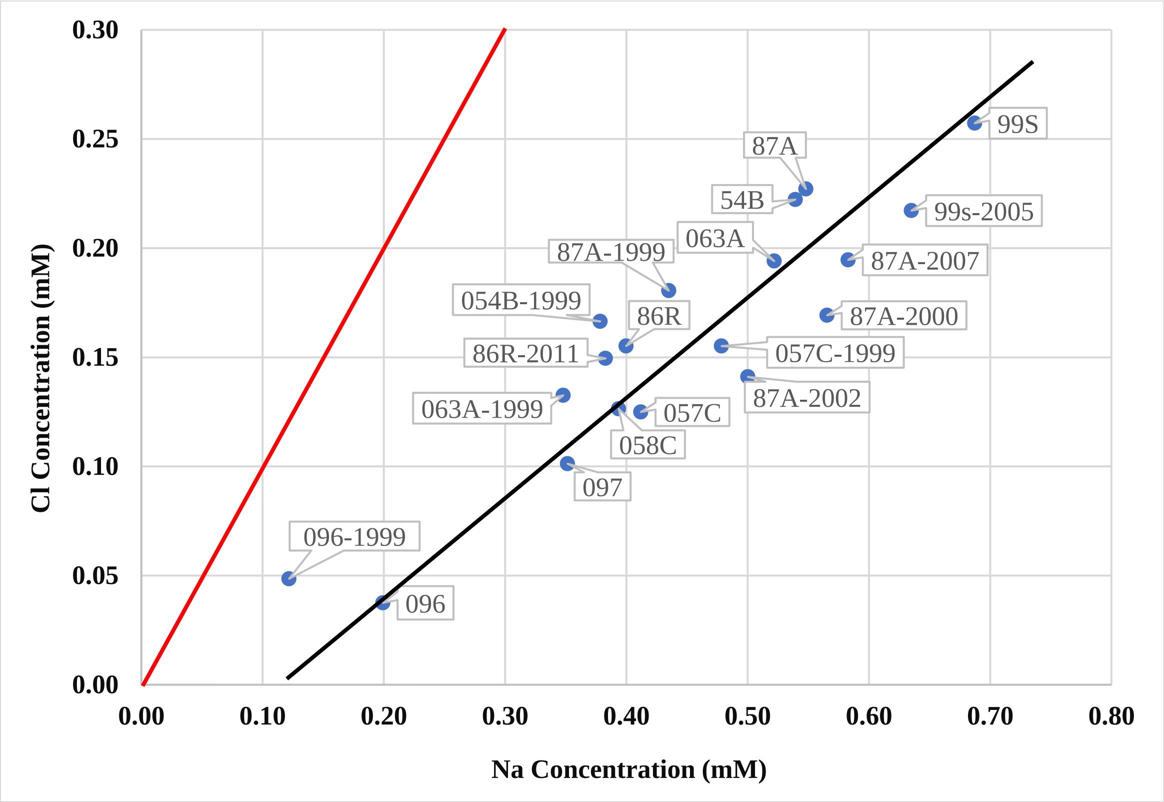

Figure 18. Molar concentration of sodium vs. chloride solute plot for samples from this study and previous studies (Larsen et al. 2003, 2016; Gentry et al. 2006). The black line represents the mixing relationship between shallow groundwater and Memphis aquifer water. The red line indicates the halite equilibrium line

Environmental Tracers

The environmental tracer data and apparent ages of Sheahan well field production well water are tabulated in Table 5. Tritium contents above 0.2 TU indicate a component of modern water (less than 60 years old), and the calculated ages are constrained by the measured tritium (Larsen et al. 2016). The tritium concentrations of most production wells sampled in July 2020 range from 0.31 to 0.74 TU, except wells 058C, 97, 96, and 99s, where values were close to or below the defined limit (0.05 TU).

Table 5. Environmental tracer data and apparent ages.

Well ID	**Aquifer**	**Sampling date**	**Top of screen depth bgs (m)**	**R/R_a**	**^{3}H (TU)**	**^{3}He (TU)**	**Age using EA (yr)**	**Age using Ne (yr)**
99s	Shallow	7/27/2020	41	1.12	bd	1.47	na*	
		08/04/2004		1.30	3.40	13.6	na	29.0
87A	Memphis	7/20/2020	95	1.14	0.74	3.77	32.4	28.7
		11/14/2007		1.14	1.0	4.8	33.0	32.0
		6/15/2005		1.11	1.60	4.70	na	24.9
		11/20/2002		1.11	1.38	4.24	na	25.2
063A	Memphis	7/13/2020	96	na	0.65	na	na*	
99	Memphis	11/3/2011	108	1.05	0.32	2.62	45	39.9
		11/19/2002		1.01	0.29	4.87	na	51.6
057C	Memphis	7/13/2020	112	1.05	0.34	1.24	27.4	na
54B	Memphis	7/20/2020	113	1.12	0.55	2.08	28.2	18.6
54B (duplicate)	Memphis	7/20/2020	113	1.12	0.46	3.15	36.8	32.8
058C	Memphis	7/13/2020	117	1.05	0.08	0.34	29.9	na
86R	Memphis	7/15/2020	130	1.10	0.31	1.54	32.0	15.5
		11/3/2011		1.02	0.36	2.17	40.2	34.9
97	Memphis	7/15/2020	144	0.96	0.21	<0	> 60	
96	Memphis	7/30/2020	211	0.80	0.03	<0	> 60	

na* due to poor gas model fit or sampling error. Here, na and bd means not applicable and below detection, respectively.

Table 5 shows the presence of modern water in the wells screened in the upper portion of the Memphis aquifer (screen top up to 130m) with an age range of 27.37 to 44.95 years using the EA method and 15.5 to 51.6 years using the Ne method. The EA model incorporates Xe gas in addition to the other noble gases and may yield robust value for ages.

To compare the measured helium-isotope to that of air-saturated water, the R/R_a ratio was calculated (Larsen et al. 2013). The R/R_a ratio (Table 5) of production well waters ranges from 0.80 to 1.30, with most wells having a ratio close to 1.

Figure 19 illustrates a comparable pattern in concentration with depth trends for both ^{3}H and Cl^{-}, indicating Cl^{-} acts conservatively, and mixing occurs between two chemically different waters, such as shallow groundwater and Memphis aquifer water. Similar phenomena were observed by Larsen et al. (2003) during fall 1999 and spring-summer 2000 sampling events in the Sheahan well field. However, the trend of decreasing tritium with depth for the summer 2020 samples is evident for all wells except for 99s which likely contains pre-modern water (Larsen et al. 2013).

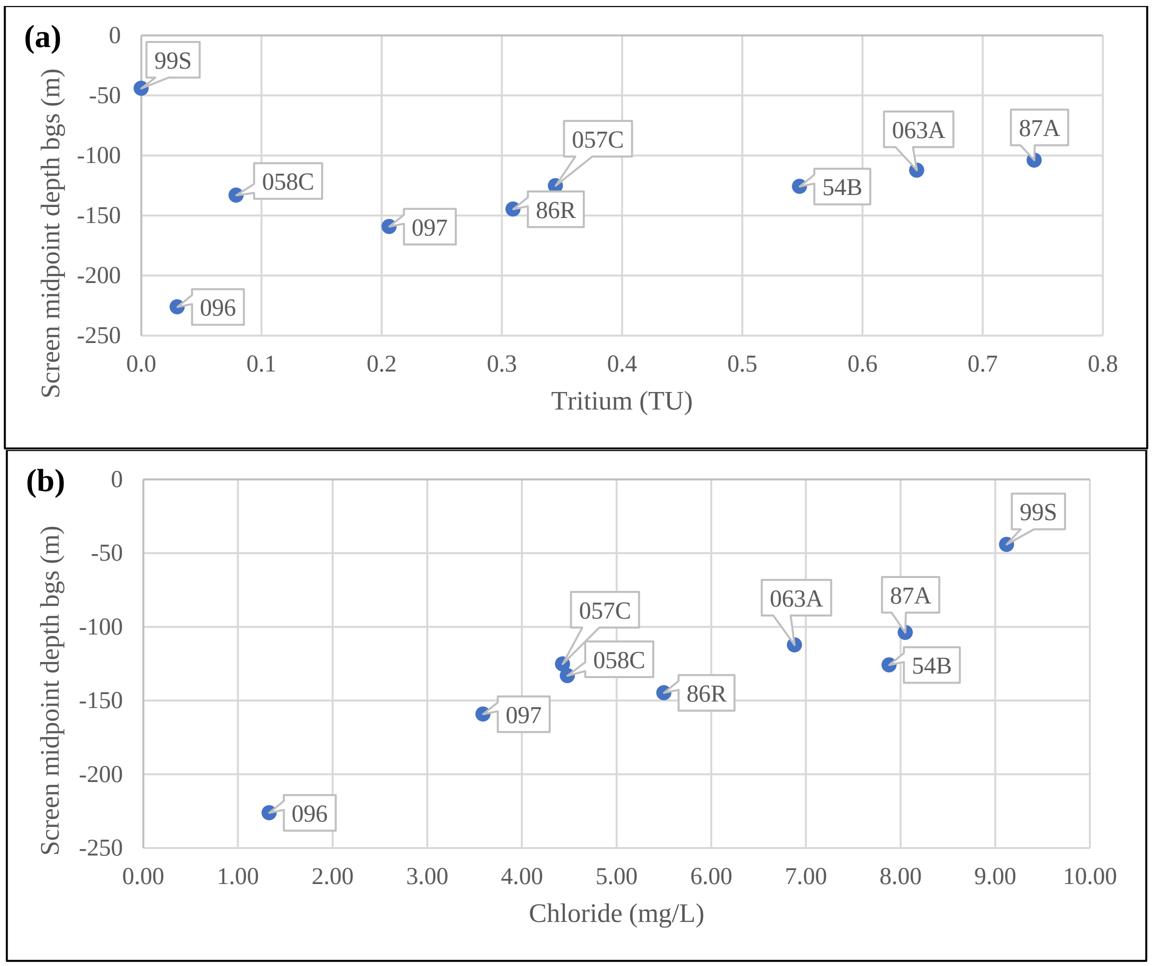

Figure 19. Plots of ^{3}H activity (a) and Cl^{-} concentration (b)screen midpoint elevation in production wells within the Sheahan well field during the Summer 2020 sampling event.

Geochemical Inverse Modeling

PHREEQCi was utilized to estimate the mixing percentages between the shallow groundwater and Memphis aquifer using geochemical data collected in the summer of 2020 at the Sheahan well field following procedures by Larsen et al. (2003, 2013, and 2016) and Koban et al. (2011). Model end members were chosen using the molar concentration plot (Figure 18) of conservative chemical species. From Figure 18, 99s and 97 were selected as the shallow (water-table) and Memphis aquifer end members, respectively. Well 97 was selected because it is centrally located within Sheahan and is screened in the most productive part of the Memphis aquifer while also having compositional similarity to other production wells (Figures 17 and 18). Well 97 also contains the least quantity of modern water, as indicated by having one of the lowest tritium concentrations (Table 5) among the other well field production wells (except wells 96 and 058C). Even though well 96 was not impacted by modern water (Table 5), it was discarded as an end member because the water quality (Figure 17 and Table 4) was likely somewhat distinct from the other wells and was screened much deeper in the Memphis aquifer. Well 058C could serve as a better end member, but it would negatively contribute to mixing models for well 97, as well 97 lies below 058C on the mixing line (Figure 6). Shallow aquifer end member 99s, though screened in the Cockfield Formation, was selected due to the historical presence of an anomalous water-table depression (Konduro-Narsimha 2007; Ogletree 2017; Lozano-Medina 2022) and modern water component (Larsen et al. 2003; 2013; Gentry et al. 2006).

Table 6. Mixing percentages and mineral reactions determined by PHREEQCi modeling**.**

Well ID (sample date)	Mixing percentages		Precipitating minerals	Dissolving minerals	Uncertainty limit	Sum of residuals
	% Shallow aquifer 99s (2020)	**% Memphis aquifer 97 (2020)**				
57C (2020)	0	100	$Fe(OH)_3$, Goethite, Hematite	Siderite, Pyrite	4.56	4.56
58C (2020)	0	100	$Fe(OH)_3$, Goethite, Hematite	Siderite, Pyrite	5.42	5.42
63A (2020)	14.28	85.72	Hematite	Siderite, Halite, Jarosite-K	10.69	8.41
86R (2020)	23.11	76.89	$Fe(OH)_3$, Goethite	Barite, Dolomite, Pyrite, CO_2(g), Rhodochrosite, Siderite	3.05	1.62
54B (2020)	14.28	85.72	Hematite	Halite, Pyrite, Jarosite-K	6.28	4.96
87A (2020)	15.53	84.47	Goethite	Pyrite, CO_2(g), Rhodochrosite, Halite	8.97	8.44

Each production well was modeled using inverse geochemical modeling as a mixture of water from wells 99s and 97, with mixing percentages tabulated in Table 6. Table 6 reports the uncertainty limits and sum of residuals for each model. A lower uncertainty limit and the sum of residuals are required to imply a model with a better fit. The maximum uncertainty limit and the sum of residuals for modeling calculations were 10.69 and 8.41, respectively, which is acceptable. Since well 96 is screened in a deeper portion of the Memphis aquifer, its tritium concentration is below the detection limit, and its water composition is dissimilar to other wells (Figure 17), this well was eliminated from the mixing model. Modeling results also included various combinations of the precipitation and dissolution of the minerals (Table 6), commonly found in the loess, shallow aquifer, UCCU, and Memphis aquifer (Larsen et al. 2013).

Production wells containing a component of modern water yielded a mixing percentage range of

14.28 to 23.11%, whereas production wells 57C and 58C lacked modern water in the mixing solution.

Lumped Parameter Modeling

The appropriate LPM was selected based on the hydrogeologic conceptualization of the local leakage process near well fields and justified by hydrogeologic and geochemical data from previous studies (Larsen et al. 2003, 2013, 2016; Koban et al. 2011; Ivey et al. 2008). Typically, a binary mixing model (BMM-EPM-DM) was found most suitable for the Sheahan well field in which one component of the mixture was modeled by using an exponential piston-flow model (EPM) and the other component modeled using a dispersion model (DM). Here, the modern water component in the shallow aquifer was modeled using EPM, where EPM ratio (EPMP) is the distance from a breach to a production well of interest (X*) divided by breach width (X), see Table 7 (Cook and Böhlke 2000; Jurgens et al. 2012). According to Larsen et al. (2016), pre-modern water component flow was modeled using a DM with a mean age of 2,000 years for the Sheahan well field. The dispersion parameter (DP) is the inverse of the Peclet number, or the ratio of dispersion coefficient (D) to the velocity (v) and outlet position (x) (Jurgens et al. 2012). The dispersion parameter (DP) was set to 0.5 following Larsen et al. (2016) for the Sheahan well field.

Table 7. Lumped parameter modeling results for the Sheahan well field.

Well ID	Sampling date	Calculated EPMP Ratio (X*/X)	LPM model	Vadose zone travel time (yr)	Mean age of modern water (yr)	Modeled EPMP	Mixing % of modern water	Mean age of pre-modern water (yr)	Tracers optimized	Relative error (%)
057C	7/13/2020	4.09	BMM-EPM-DM	25.0	2.97	5.70	14.3%	2000	^{3}H, ^{3}He(trit)	6.62%
058C	7/13/2020†	3.75	BMM-EPM-DM	25.0	2.00	3.27	3.69%	2000	^{3}H, ^{3}He(trit)	217%
063A	7/13/2020	5.26	BMM-EPM-DM	25.0	19.0	5.16	9.60%	2000	^{3}H	0.00%
97	7/15/2020	5.81	BMM-EPM-DM	25.0	9.10	7.66	8.50%	2000	^{3}H	0.00%
86R	7/15/2020	8.33	BMM-EPM-DM	25.0	10.3	8.92	12.0%	2000	^{3}H, ^{3}He(trit)	0.00%
	11/3/2011†		BMM-EPM-DM	25.0	9.5	8.73	11.0%	2000	^{3}H, ^{3}He(trit)	220%
54B	7/20/2020	6.58	BMM-EPM-DM	25.0	15.1	6.07	11.9%	2000	^{3}H, ^{3}He(trit)	0.00%
87A	7/20/2020	6.93	BMM-EPM-DM	25.0	23.2	6.86	7.01%	2000	^{3}H, ^{3}He(trit)	0.03%
	11/14/2007		BMM-EPM-DM	25.0	27.2	7.34	8.00%	2000	^{3}H, ^{3}He(trit)	8.41%
	6/15/2005		BMM-EPM-DM	25.0	21.1	6.18	6.06%	2000	^{3}H, ^{3}He(trit)	0.02%
	11/20/2002		BMM-EPM-DM	25.0	21.4	7.49	7.09%	2000	^{3}H, ^{3}He(trit)	0.09%
96	7/30/2020	14	BMM-EPM-DM	25.0	11.7	13.4	1.01%	2000	^{3}H	0.00%
99	11/3/2011	1.0	BMM-EPM-DM	25.0	34.4	2.64	4.10%	2000	^{3}H, ^{3}He(trit)	0.00%
	11/19/2002		BMM-EPM-DM	25.0	28.7	2.80	8.00%	2000	^{3}H, ^{3}He(trit)	55.7%
99s	7/27/2020†	1.0	BMM-EPM-DM	25.0	7.45	2.26	2.50%	2000	^{3}He(trit)	0.00%
	6/3/2004		BMM-EPM-DM	25.0	22.1	2.66	7.88%	2000	^{3}H, ^{3}He(trit)	47.3%

† Questionable model based on relative error or the use of only ^{3}He for optimization.

Another important parameter in LPM modeling is the travel time in the paleochannel and shallow aquifer before entering the breach. In the Sheahan well field, water from Nonconnah Creek travels through the shallow aquifer along a paleochannel acting as a conduit before infiltrating into the Memphis aquifer through breaches (Figure 16) (Larsen et al. 2013; Torres-Uribe et al. 2021). To calculate travel time, it is necessary to know the hydraulic gradient between Nonconnah Creek and a shallow monitoring well at the breach location and the horizontal hydraulic conductivity of paleochannel materials. During the sampling event in the summer of 2020, the hydraulic head at a monitoring well 99s was 15.4 m below that of Nonconnah Creek, which flows east to west approximately 4.5 km south of well 99s. The horizontal hydraulic conductivity of paleochannel material was determined to be 39.01 and 41.76 m/day using the Hazen (modified) and Wang et al. (2017) methods, respectively. A grain size analysis (Figure A6, Appendix-A) was performed on the core returns at 99s2 from the top of the UCCU (Cockfield Formation; 22.5 m depth below ground surface) to determine the hydraulic conductivity utilizing empirical formulas. Rosas et al. (2014) recommended the Hazen (modified) method for calculating hydraulic conductivity in river sediments, whereas Chandel et al. (2022) stated that the method described by Wang et al. (2017) could provide more accurate hydraulic conductivities based on the effective dimension (D_{10}) of the sample. With an effective porosity of 0.3 for sand and gravel (Anderson et al. 2015), the average unsaturated zone travel time for Nonconnah Creek water migrating through the paleochannel to the known breach at 99s2 was estimated to be about 25 years.

LPM models optimized with tracer data fit well for most production wells with a mixing percentage range of 1.01 to 14.3% (Table 7). Nonetheless, mixing models of wells 58C, 99s, and

86R for 2020 and 2011 were questionable due to high model error (>100%) or the use of only ^{3}He for optimization. Again, model parameters and unsaturated zone travel time derived from the 2020 data were used with historical tracer data from Larsen et al. (2016) to fit LPM models.

Comparative Assessment of the MT3DMS Results

MT3DMS was used to simulate groundwater flow and mass transport to find the mean age and mixing percentage at the sampled well locations during the Summer of 2020. The comparative analysis of mixing percentage and mean age of modern water using MT3DMS, LPM modeling, geochemical inverse modeling, and age-dating results is presented in Table 8.

Table 8. Numerical and Geochemical comparison of percentage and age of modern water for sampled wells during Summer 2020.

Well ID	Aquifer	Top of screen depth (m)	Sampling date	Age range using EA and Ne (yr)	Apparent age MT3DMS (yr)	% Modern LPM	% Alluvial Geochem	% Modern MT3DMS	% *Modern MT3DMS
057C	Memphis	112	7/13/2020	27.4	28.3	14.3	nd	15.5	15.3
058C	Memphis	117	7/13/2020	29.9	16.6	3.69	nd	2.79	3.54
063A	Memphis	96	7/13/2020	na	14.7	9.60	14.28	5.20	11.9
97	Memphis	144	7/15/2020	> 60	20.9	8.50	na	0.00	7.50
86R	Memphis	130	7/15/2020	15.5 - 32.0	14.8	12.0	23.11	0.00	6.89
54B	Memphis	113	7/20/2020	18.6 - 36.8	36.0	11.9	14.28	9.40	9.60
87A	Memphis	95	7/20/2020	28.7 - 32.4	26.0	7.01	15.53	0.20	0.50
96	Memphis	211	7/30/2020	> 60	50.2	1.01	nd	0.0	0.0
99s	Shallow	41	7/27/2020	na	7.22	2.50	na	9.07	6.67

*Modern MT3DMS results from the transport model with an additional breach near Sh:K-099. Here, na and nd means not applicable and not detection, respectively.

The mixing fraction determined by the MT3DMS model yields modern water between 0.2 to 15.5%. Although the mixing fractions determined by LPM and MT3DMS are comparable, certain results, such as 97, 86R and 87A, produce significantly different mixing fractions. Simulating the transport model with the addition of a new potential breach (Figure 16) near

Sh:K-099 results in a mixing percentage at 97 and 86R. Although the geometry and extent of this additional breach are uncertain, the MT3DMS model with this additional breach predicts a mixing percentage between 0.5% and 15.3%.

Discussion

Conceptual hydrogeologic model

Potential pathways for local recharge of modern water to the Memphis aquifer are identified through analysis of hydrostratigraphy and water level data from the monitoring wells. The contour map of the aggregate thickness of confining clay in UCCU (Figure 16) depicts a paleochannel configuration in the center of the well field. Using a maximum thickness of 3 m of clay to designate suspected breach locations, three breaches at 99s2, FCCMW19/FCCMW20, and 78B (Figure 16) were detected within the UCCU instead of the breach identified by Parks (1990). Also, Hasan et al. (2022) used the electrical resistivity method to interpret the presence of an additional potential breach near Sh:k-99 (Figure 16), which is an E-W extension of the paleochannel feature at FCCMW19/FCCMW20, and 99s2. The potential breaches at 78B and Sh:k-99 require additional drilling for verification. The absence of a laterally continuous confining clay at boreholes 99s2, FCCMW19/FCCMW20, 78B and close to Sh:k-099 due to an erosional remnant of paleochannel traversing the Sheahan well field. These breaches were utilized to construct the CAESER-II groundwater-flow model, which improved the flow model at Sheahan well field.

Borehole 99s2 and monitoring well FCCMW06 revealed that the fluvial-terrace deposits were unsaturated. Instead, the zone of saturation was found between 30 and 38 meters below the ground surface, beneath the fluvial-terrace deposits in the Cockfield Formation (cross-sections A-A′ and D-D′). Hence, it is the presence of a UCCU breach at these two locations, plus their proximity to the Sheahan well field and subsequent major production from the Memphis aquifer (0.13 million m^3/day), that has likely depleted the fluvial-terrace (shallow) aquifer.

In addition, water level measurements (Figure A7, Appendix-A) were taken from shallow, Memphis aquifer monitoring wells in and around the Sheahan well field and Nonconnah Creek in July 2020. The water-table surface showed an anomalous depression on the west side of the Sheahan well field around Sh:K-163 (99s) (Figure A7(a), Appendix A), which matches a previous study by Larsen et al. (2013) and later shown in Lozano-Medina (2022). No extensive withdrawals are known to occur from the shallow aquifer in this area that could result in water level depressions. Additionally, Memphis aquifer heads are lower than the water-table, suggesting downward vertical leakage, a pattern also seen elsewhere in Shelby County (Parks 1990; Bradley 1991; Carmichael et al. 1997, 2018; Konduro-Narsimha 2007; Ogletree 2017; Smith 2018). In the case of the shallow aquifer, the general gradient of the shallow aquifer under Sheahan would tend to go south towards Nonconnah Creek, but instead, a pronounced lateral gradient is present going from the creek towards the well field and Sh:K-163 (99s) (Konduro-Narsimha 2007; Larsen et al. 2013; Ogletree 2017; Lozano-Medina 2022). Hence, the potential leakage pathway from Nonconnah Creek to the Sheahan well field is interpreted along the paleochannel formed by erosional and depositional processes of fluvial-terrace material atop the UCCU, as suggested by Larsen et al. (2013), as well as leakage through the four hydrologic breaches in the UCCU related to a potential Eocene paleochannel system designated in this paper.

Geochemical evidence for mixing

Several geochemical indications of groundwater leakage through the UCCU in Memphis aquifer production wells in the Sheahan well field are apparent. A higher concentration of Na^+, Cl^-, NO_3^-, SO_4^{2-}, Fe and specific conductance was detected in the water of production well 54B compared to other wells with a comparable screen depth. Production well 54B may receive shallow groundwater containing elevated concentrations of Na^+, Cl^-, NO_3^-, and SO_4^{2-} from two nearby breach locations: the known breach at the FCC site and a suspected breach at 78B.

Piper plot (Figure 17) shows the composition of 99s is more Na+K rich than the Memphis aquifer, but the bicarbonate content is comparable to that of the Memphis aquifer, indicating a mixing relationship consistent with previous studies (Larsen et al. 2003, 2013; Ivey et al. 2008). Moreover, the shallow groundwater composition in 99s plots along the linear array with cations for Memphis aquifer water but with higher Na+K (Figure 17), which again is consistent with mixing due to UCCU leakage. On the other hand, Larsen et al. (2013) described a substantial amount of Nonconnah Creek water in wells 99s and 96s. Larsen et al. (2003) also found elevated concentrations of Na^+, Cl^- and SO_4^{2-} present in Nonconnah Creek, comparable to those in upper Memphis aquifer wells and shallow groundwater in observation wells. Again, the piper plot with historical data (Figure A4, Appendix-A) shows shallow aquifer well (96s) plots on the cations triangle along the linear array with 99s, whereas the shallow groundwater (99s and 96s) and creek water composition have similar bicarbonate. Therefore, the chemistry of the water in wells 96s and 99s is interpreted as being closely related to that of the water in Nonconnah Creek. Thus, the geochemical data are consistent with Nonconnah Creek water migrating down-gradiaent along a post-Eocene paleovalley feature and entering monitoring wells (96s and 99s) through breaches, which explains the overall mixing relationship between shallow groundwater beneath the Sheahan well field and Nonconnah Creek water.

Cross-plots of solute concentrations detect geochemical trends in the water of sampled wells, which also indicates a mixing relationship. The cross-plot of sodium versus chloride (Figure 18) shows that well 99s is at one end of the trend line of groundwater in the Memphis aquifer, suggesting mixing occurs between shallow groundwater at 99s and Memphis aquifer wells. Hence, 99s is a source of recharge to the Memphis aquifer.

PHREEQCi geochemical inverse modeling results show the mixing percentage of modern water in Sheahan well field waters. The model of wells 57C and 58C yielded no evidence of modern water. The model result is consistent with the fact that both 57C and 58C are screened at a similar depth and plot near end member 97 on the mixing line (Figure 18), indicating a greater contribution of Memphis aquifer water. In addition, the absence of alluvial water in the mixing solution for 58C is consistent with tritium activity close to the detection limit (Table 6).

Larsen et al. (2016) conducted geochemical inverse modeling at multiple wells in the Sheahan well field (sampled in 2000, 2002, 2007 and 2011); among these wells, well 87A and 86R can be compared to the current modeling effort as they were resampled in 2020. In 2000 and 2002, the mixing proportion at well 87 was determined to be 12 and 22%, respectively, but no geochemical mixing model was identified during the 2007 sampling. Similarly, during the 2011 sampling event, there was no mixing model for well 86R. However, the 2020 mixing percentages at wells 87 and 86R were 15.53% and 23.11%, respectively (see Table 6). Different end members could account for the difference in mixture percentage compared to previous modeling results. Gallo et al. (2015) found that selecting different end members with slightly different chemical properties could result in substantially different mixing fractions.

Environmental tracer evidence for mixing

Environmental tracers are another indicator for vertical groundwater leakage through aquitard breaches in the Sheahan well field. Historical data (Table 5) for production wells 87A, 99, and 86R indicate that ^{3}H, ^{3}He, and apparent ages have remained relatively constant, within the error of apparent age analysis, throughout the years. This may account for the dynamic equilibrium between pumping and leaking. Nonetheless, seasonality may account for the slight variation, as Larsen et al. (2003) found that fall sampling events typically had higher activity than spring and summer events.

In contrast, well 99s, located on the same property lot (1845 m^2) as 99s2, did not contain tritium during the 2020 sampling event. This is because the breach at well 99s may not be hydrogeologically well connected to the subsurface paleovalley systems or inconsistent pumping conditions from well 99 (same lot). Interestingly Larsen et al. (2013) reported that 99s, sampled in August 2004, contained older helium-3-rich water; thus, it may contain a substantial amount of pre-modern water.

R/R_a ratio close to 1 indicates the presence of young water, whereas a value greater than 1 indicates an older sample (Larsen et al. 2013). Again, $R/R_a < 1$ indicates that the helium content of wells has been affected by mixing with older and deeper groundwater sources (Larsen et al.

2016). Except for the deep-screened production well 96 and the shallow well 99s, the R/R_a values for most wells are close to 1, which is consistent with atmospheric helium values and indicates the presence of young water (Cook and Herczeg 2000; Gallo 2015).

LPM modeling also determined age distributions and mixing fractions of modern water produced from Sheahan well field production wells. LPM considers the contributions of modern water from the 1960s or later; consequently, age distributions of 60 years typically produce a younger mean age than $^3H/^3He$ apparent ages (Larsen et al. 2016; Cook and Bohlke 2000). Although the breach shape is uncertain (Torres-Uribe et al. 2021; Ivey et al. 2008), the calculated and modeled EPMP ratios based on Figure 16 were in close agreement and well-constrained by the hydrogeologic cross-section data (Figure 10).

Table 7 shows a few mixing models with high relation error, which may be attributed to low $^3H/^3He$ content in the sampled wells, or alternative LPM parameters may be required. Additionally, model parameters and unsaturated zone travel time derived from the 2020 data appear to yield models with low to moderate error for the historical tracer data from Larsen et al. (2016). In 86R and 87A, there is no significant trend in mixing fractions over the course of almost 20 years, indicating a dynamic equilibrium between modern water leakage and pumping in the aquifer. Also, historical water level data from the U.S. Geological Survey National Water Information System (NWIS) and recently installed pressure transducer data at 99s indicate that groundwater levels have steadily risen by more than 8 m between 2002 and 2020. Thus, the decrease in hydraulic gradient between Nonconnah Creek and 99s has led to a decrease in the discharge of shallow groundwater water in recent years, as both wells 99 and 99s have exhibited less modern water.

Apparent age of modern water and mixing percentage

Comparative analysis (Table 8) of LPM and MT3DMS modeling yields comparable results for mixing percentage for the 2020 sample of production wells. However, well 87A shows a different mixing percentage between LPM and MT3DMS results. The significant mixing fraction difference at 87A might account for the missing hydrogeologic connection in the groundwater model on the eastern part of the well field, where few control points are available for hydrogeologic interpretation. The tracer data used for LPM modeling represents a point measurement of groundwater mixing, typically during periods of the year with significant pumping demand. Consequently, LPM models may overestimate the mixing fraction and could represent the highest level of mixing. Also, the accurate conceptualization of the EPM ratio (X*/X) could constrain the mixing percentage close to the estimate obtained from MT3DMS. On the other hand, geochemical mixing models are sensitive to the chemical properties and selection of end members (Larsen et al. 2016). Therefore, the mixing percentage derived with PHREEQCi could be re-evaluated by sampling different shallow aquifer end members, as different end members may contain varying amounts of modern water (e.g., Gallo 2015).

Similarly, estimates for the apparent age of the modern water derived from MT3DMS lie within the age range for most wells obtained from environmental tracers ($^{3}H/^{3}He$ age), except for well 96. Tracer-based apparent ages may be affected by mixing waters of various ages in a field-collected groundwater sample, sometimes including water with ages greater than 60 years

(Andersen et al. 2015). However, MT3DMS considers modern water's contributions from the 1960s or later; as a result, age distributions are circumscribed by only 60 years, which could result in apparent ages that differ from tracer-based ages. Moreover, the $^{3}H/^{3}He$ system is highly sensitive to mixing, and precise age estimates require short well screens (Cook 2020). Another complicating factor is the potential for helium loss during the sampling event, resulting in a $^{3}H/^{3}He$ apparent age bias towards older ages (Larsen et al. 2016).

However, if the cell size were reduced from 250 m to a smaller value and if additional vertical layers were included, the MT3DMS model could more accurately capture the movement of modern water through geological layers and provide more accurate estimates of mixing percentage and mean ages. In addition, the longitudinal and transverse dispersivity could be heterogeneous rather than constant, as presumed in this study, and spatially variations could yield more accurate estimate of the proportion of mixing and apparent ages. In addition, implementing additional surface processes such as adjusting areal recharge, evapotranspiration, and tributary streams could improve the modeling of shallow unconfined aquifer (Pierce 2022) and thus more accurately represent the mixing percentage and mean age obtained from the MT3DMS model.

Conclusion

This study utilized hydrostratigraphic, hydrogeologic, geochemical, environmental tracer, and numerical modeling data to determine the sources, pathways, and mixing percentage of modern water contributing to production wells at the Sheahan well field.

Hydrogeologic cross-sections conceptually identified likely recharge pathways of modern water from the shallow aquifer to the underlying Memphis aquifer. Cross-sections indicated the likely presence of multiple breaches in the UCCU at boreholes 99s2, 78B, FCCMW19/FCCMW20, and near Sh:k-099 resulting in a hydraulic connection between the shallow and Memphis aquifers.

The elevated Na^+ and Cl^- concentrations in the shallow groundwater and upper Memphis wells, which decrease with depth, indicate a mixing relationship between water from the shallow aquifer and water from the Memphis aquifer, especially in the upper part of the Memphis aquifer. Geochemical data show linear arrays for both conservative and non-conservative major solutes in shallow and Memphis aquifer groundwater, suggesting a mixing relationship. In addition, cross-plots (sodium vs. chloride, alkalinity vs. calcium, and magnesium vs. calcium) reveal a linear mixing trend between all production wells and shallow groundwater. Environmental tracers (^3H and ^3He) produced from the 2020 sampling event were combined with historical tracer data to evaluate the presence and estimated ages of modern water in the Memphis aquifer at the Sheahan well field. Tritium data for most wells indicate the presence of modern water except wells 58C, 97, 96, and 99s, where tritium levels were near or below 0.2 TU. The apparent $^3H/^3He$ ages of affected wells lie within the range of 27.37 to 44.95 years using the EA method and 15.5 to 51.6 years using the Ne method. Tritium-based groundwater age estimations can be unreliable, especially for younger ages, because the $^3H/^3He$ system is more sensitive to older modern water. The consistency of water quality and tracer data over the course of 20 years indicates a dynamic equilibrium condition between pumping and leakage. However, the variation in some wells as a result of a decline in production or variation in shallow aquifer saturation.

Inverse geochemical mixing models using 99s as the shallow end member and 97 as the Memphis aquifer end member indicate that the quantity of shallow aquifer water mixed with Memphis aquifer water in production wells ranged between 14.28 and 23.11%. However, inverse geochemical modeling is sensitive to the selection of end members. In addition, a lumped parameter model (BMM-EPM-DM) was fitted to the tracer data to determine the mean age and mixing percentage of modern water. The LPM model optimized with tracer data generated a mixing percentage ranging from 1.01 to 14.26% in the production wells. LPM models are binary mixing models and typically produce a younger mean age than the $^{3}H/^{3}He$ apparent ages. The MT3DMS model was used to estimate the apparent mean age and mixing percentage of individual production wells sampled in the Summer of 2020. The apparent age of modern water derived from MT3DMS fell within the range of the apparent ages of $^{3}H/^{3}He$, except for well 96. However, the age distributions from the MT3DMS model are limited to 60 years or less, resulting in a younger mean age than the tracer-based apparent ages. Again, MT3DMS determined that as much as 15.52% of modern water was extracted from the Memphis aquifer in affected wells. The LPM modeling mixing percentage closely matches MT3DMS results except for 87A, which may indicate a lack of hydrogeological connection on the eastern well field. Both LPM and MT3DMS modeling required accurate hydrogeologic conceptualization to have a better estimate. Since LPM modeling may overestimate the mixing fraction and inverse geochemical modeling is sensitive to the selection of end members, the MT3DMS mixing percentage is more representative of the Sheahan well field.

The modeling strategy used here presents an ideal tool that can be used to predict how modern water and Memphis aquifer water will mix over time along subsurface flow paths. Thus, MODFLOW and MT3DMS simulations can be coupled with long-term tracer data to validate the transport model while estimating the mean age and mixing percentage of modern water in the Memphis aquifer, thereby ensuring the long-term sustainability of a well field.

SUMMARY AND CONCLUSION

The existing Shelby County groundwater flow model (CAESER-I) was updated and re-calibrated to simulate the groundwater flow dynamics within individual hydrostratigraphic units. Although the model is consistent with the base model (CAESER-I), the modified version (CAESER-II) improves upon by addressing some of the shortcomings identified by Torres-Uribe et al. (2021) and Villalpando-Vizcaino et al. (2021). Thus, CAESER-II model will be used for predictive simulations and may eventually be coupled with the flow model to simulate contaminant transport.

Hydrogeologic cross-sections conceptually identified likely recharge pathways of modern water from the shallow aquifer to the underlying Memphis aquifer. Known breaches were confirmed through core samples in the center of the wellfield (99s2) and to the west near Highland and Southern Avenues (FCCMW19/FCCMW20).

Water quality and tracer data consistency over 20 years indicates a dynamic equilibrium between pumping and leakage. Elevated Na^+ and Cl^- concentrations in the shallow groundwater and upper Memphis wells indicate a mixing relationship between the shallow and Memphis aquifer, these concentrations decrease with depth. Additional, geochemical analyses and mixing models show similar mixing relationships between water from the shallow and upper Memphis aquifer. Inverse geochemical mixing models indicate that the quantity of shallow aquifer water mixed with Memphis aquifer water in production wells ranged between 14.28 and 23.11%. The lumped parameter model (LPM) optimized with tracer data generated a mixing percentage ranging from 1.01 to 14.26% production wells with evidence of modern water.

Historical and current environmental tracer ^{3}H (tritium) and ^{3}He (helium-3) data indicate the presence of modern water except production wells 58C, 97, and 96, and "shallow" aquifer observation well 99s, where tritium levels were near or below the detection limit. The apparent $^{3}H/^{3}He$ ages of affected wells lie within the range of 15.5 to 51.6 years old, depending on the method used. The variation in these results could be from a decline in production or variation in shallow aquifer saturation.

The MT3DMS model was used to estimate the apparent mean age and mixing percentage of individual production wells sampled in the summer of 2020. MT3DMS determined that as much as 15.52% of modern water was extracted from the Memphis aquifer in affected wells except 96. The apparent age of modern water derived from MT3DMS fell within the range of the apparent ages of $^{3}H/^{3}He$, except for well 96. However, the age distributions from the MT3DMS model are limited to 60 years or less, resulting in a younger mean age than the tracer-based apparent ages. Also, the LPM mixing percentage closely matches MT3DMS results except for 87A, which may indicate a lack of hydrogeological connection east of the well field. Since LPM modeling may overestimate the mixing fraction and inverse geochemical modeling is sensitive to the selection of end members, the MT3DMS mixing percentage is more representative of the Sheahan well field. Thus, MODFLOW and MT3DMS simulations can be coupled with long-term tracer data to validate the transport model while estimating the mean age and mixing percentage of modern water in the Memphis aquifer, ensuring the long-term sustainability of the Sheahan well field.

In the future, the MODFLOW and MT3DMS model could be improved by incorporating as much hydrogeologic conceptualization as possible. In addition, if the cell size were reduced from

250 m to a smaller value and additional vertical layers were included, the MT3DMS model could more accurately capture the movement of modern water through geological layers and provide estimates of mixing percentage and mean ages. Longitudinal and transverse dispersivity values could be heterogeneous rather than presumed to be constant across space to have a more accurate estimate of the proportion of mixing and apparent ages. Implementing additional surface processes such as adjusting areal recharge, evapotranspiration, and tributary streams could improve the modeling of shallow unconfined aquifer and thus more accurately represent the mixing percentage and mean age obtained from the MT3DMS model.

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Appendix-A

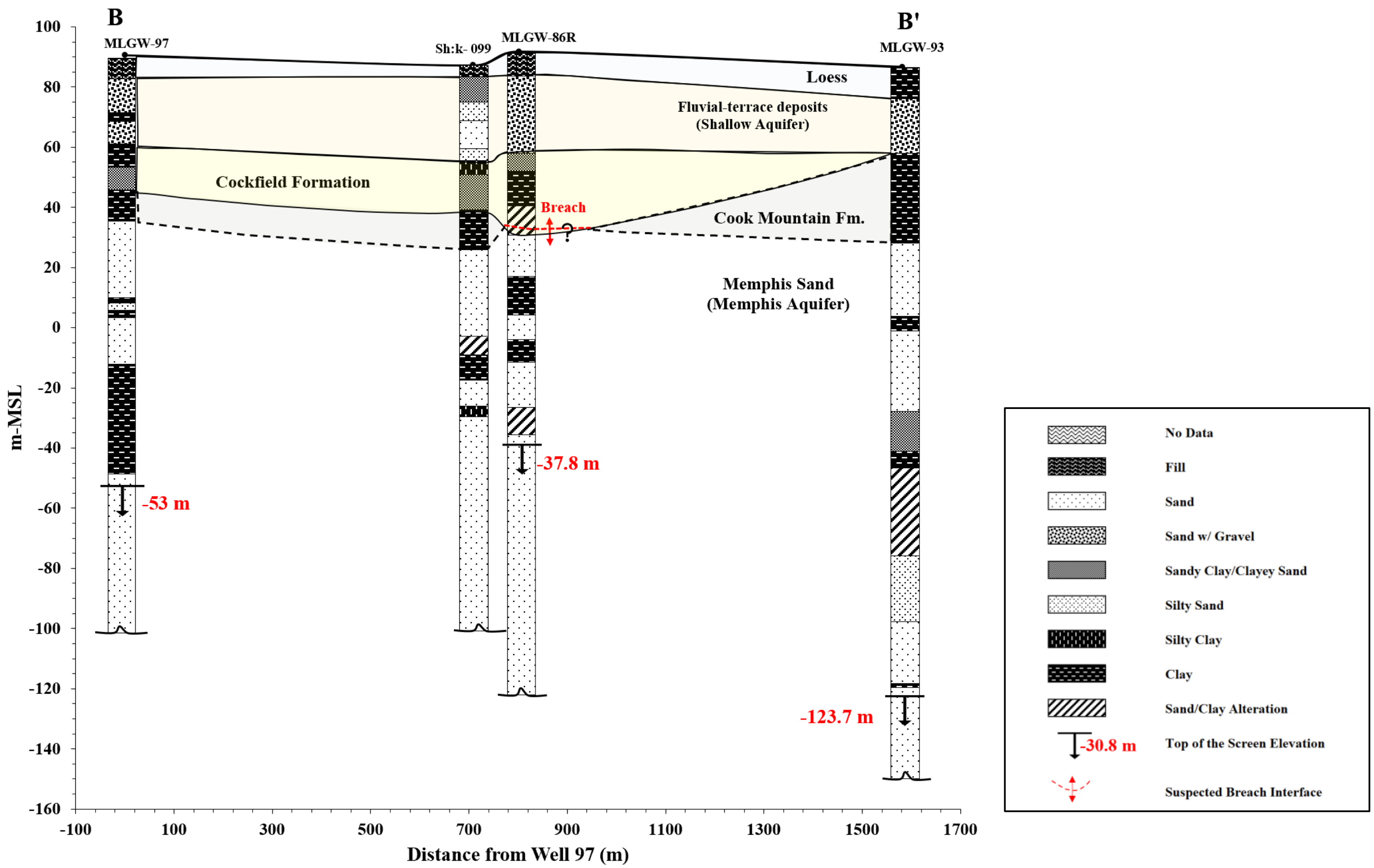


Figure A1. Cross section B-B' displays the hydrostratigraphy from north to south through the eastern part of the Sheahan well field.

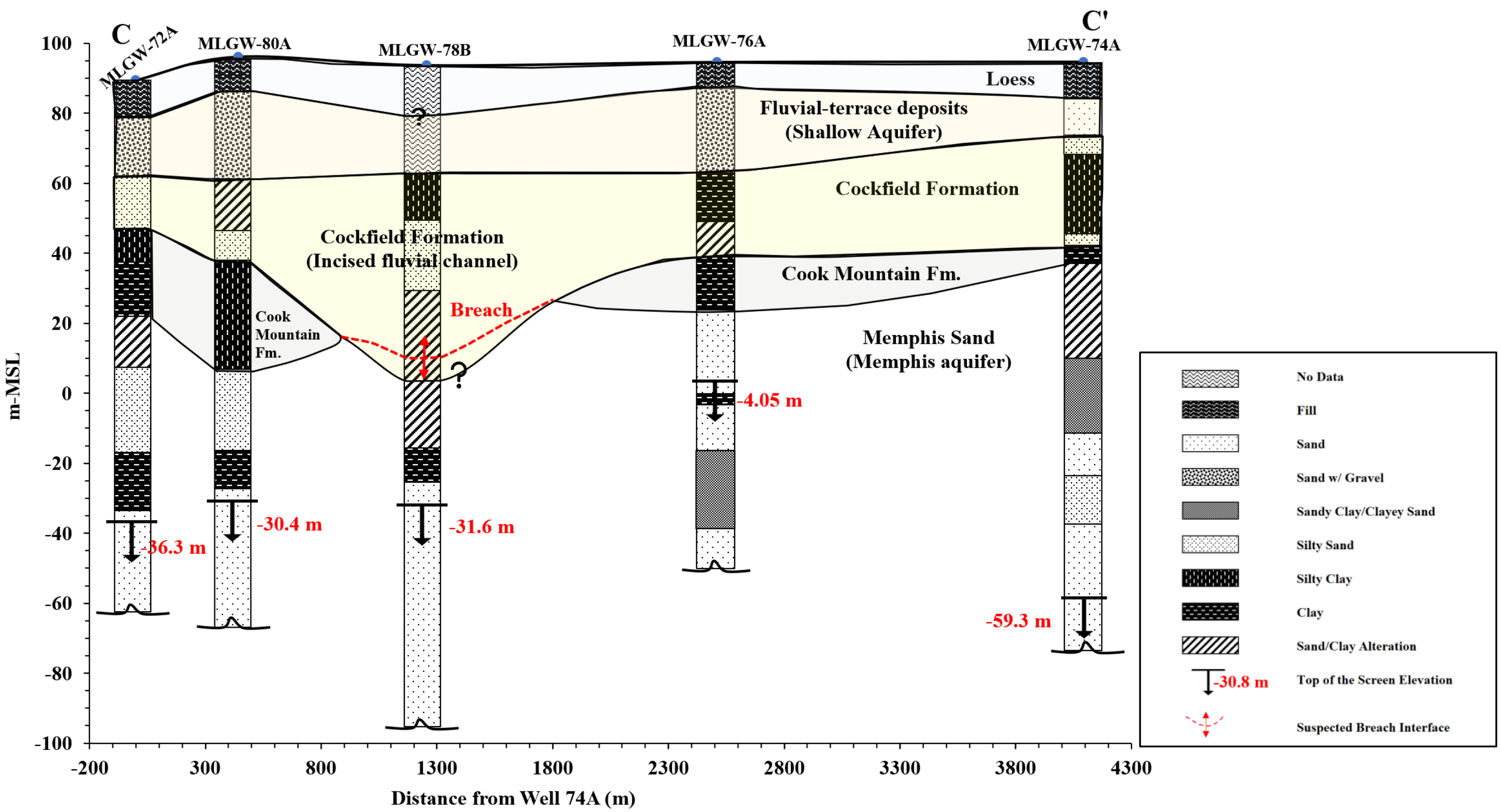


Figure A2. Cross section C-C' displays the hydrostratigraphy from west to east through the northern part of the Sheahan well field.

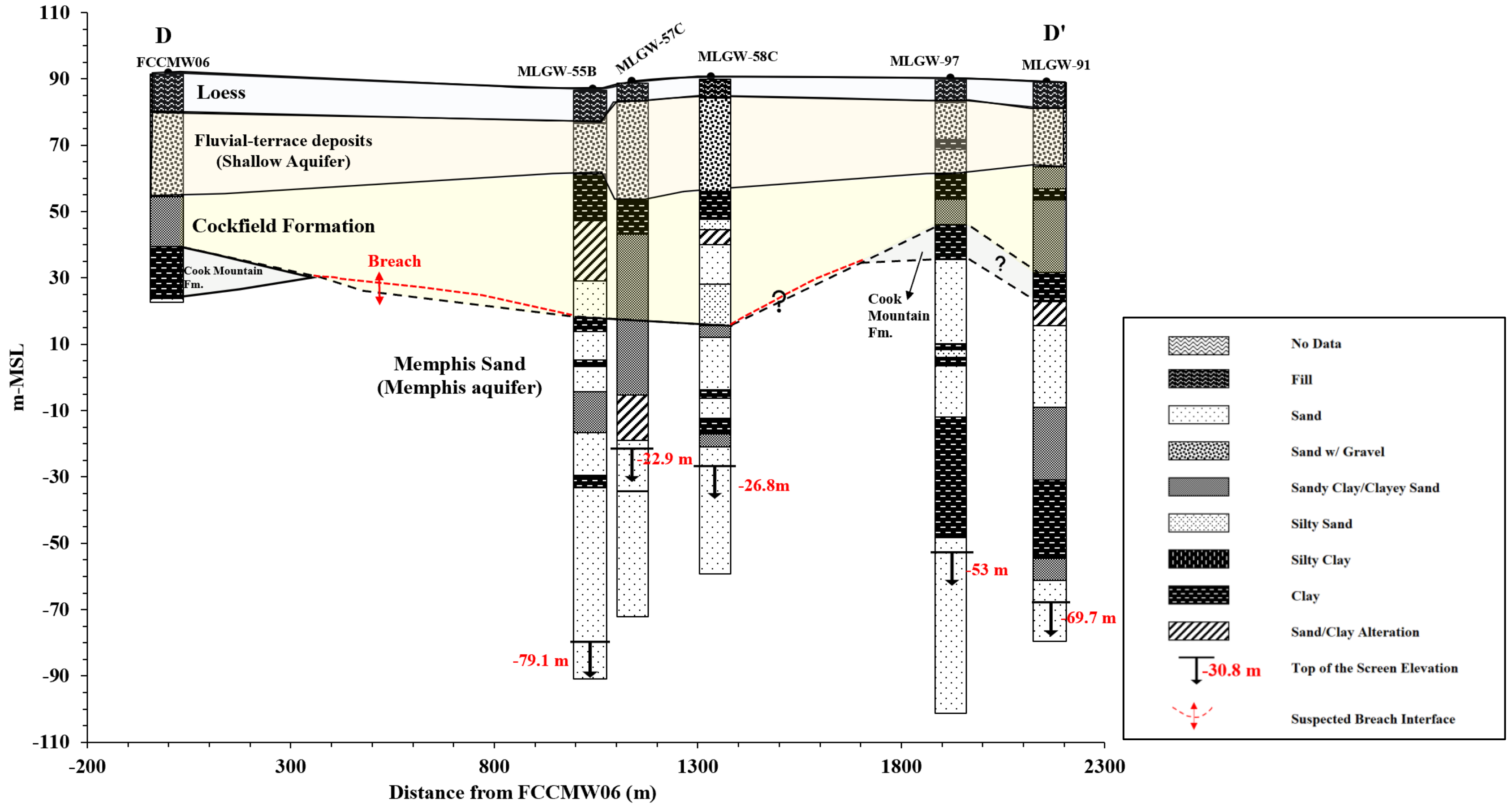


Figure A3. Cross section D-D' displays the hydrostratigraphy from west to east through the middle part of the Sheahan well field.

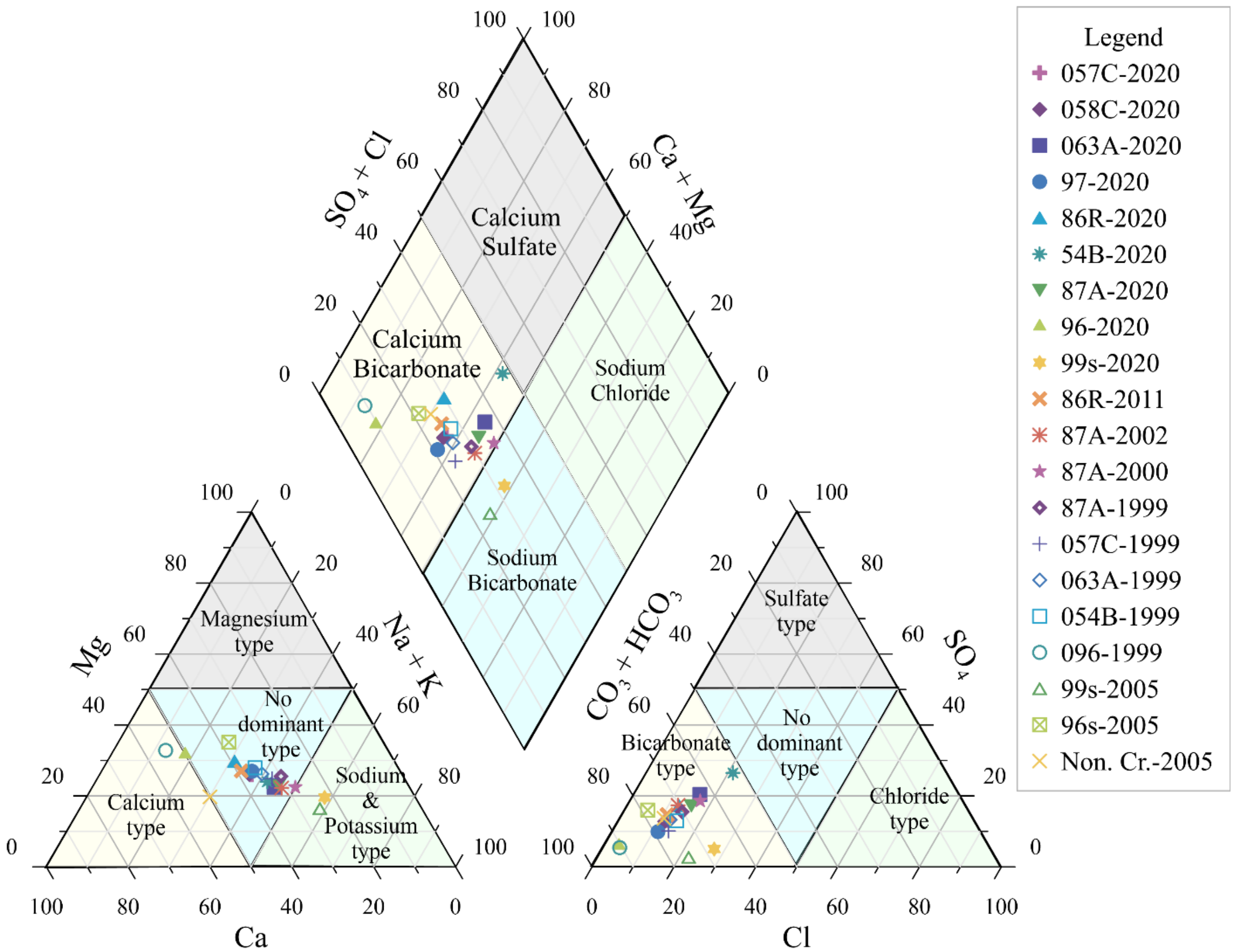
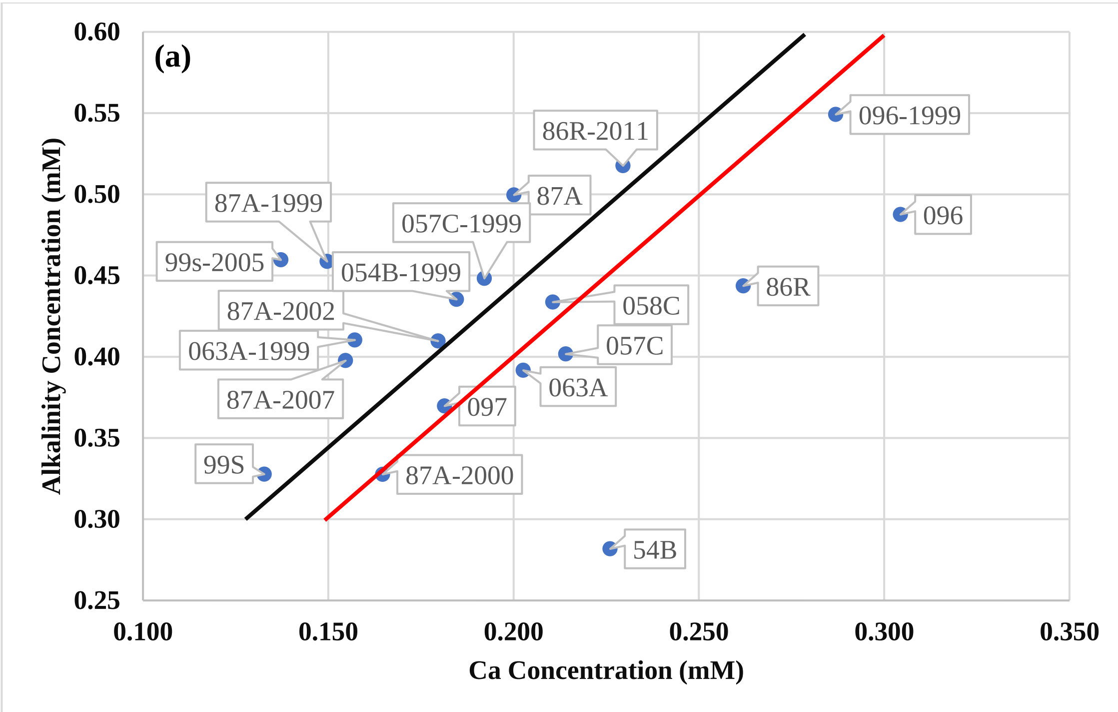


Figure A4. Piper diagram showing hydrochemical water types for Sheahan well field groundwater samples from 1999, 2000, 2002, 2005, 2011 and 2020. Here, Non. Cr. is Nonconnah Creek water point and 96s (Sh:K-156) is shallow monitoring well shown in Figure A7 (Appendix-A).



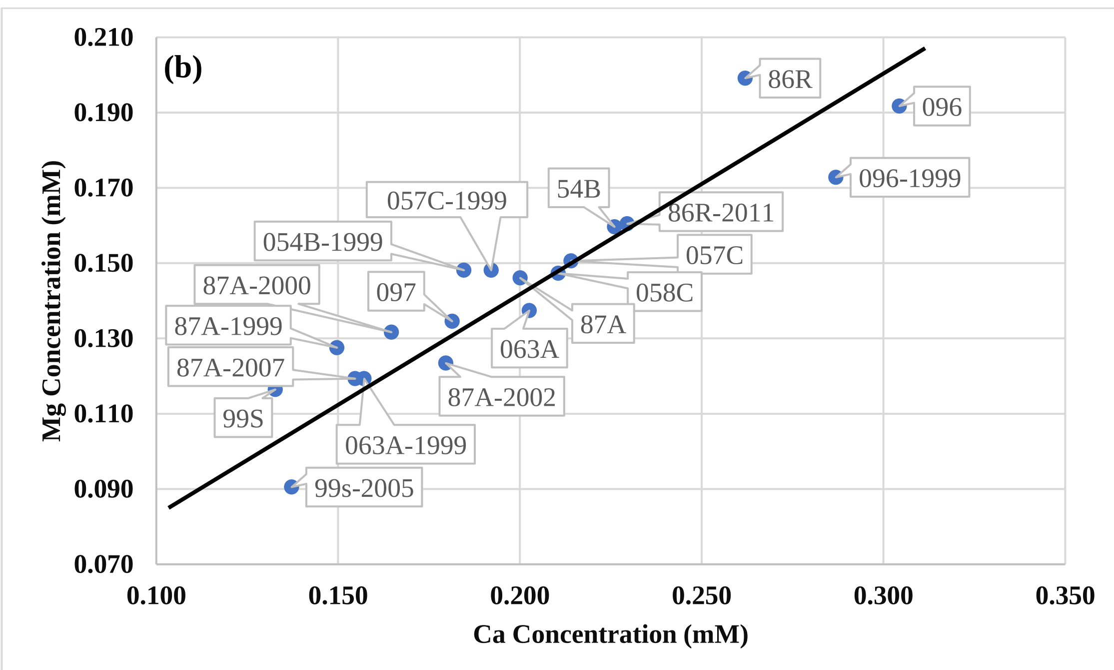


Figure A5. Molar concentration solute plot for samples from this study as well as from previous studies (Larsen et al. 2003, 2013; Gentry et al. 2006). (a) alkalinity vs Calcium (b) magnesium vs calcium. The black line represents the mixing relationship between shallow groundwater and Memphis aquifer water. The red line indicates dolomite equilibrium line (Figure A5(a)).

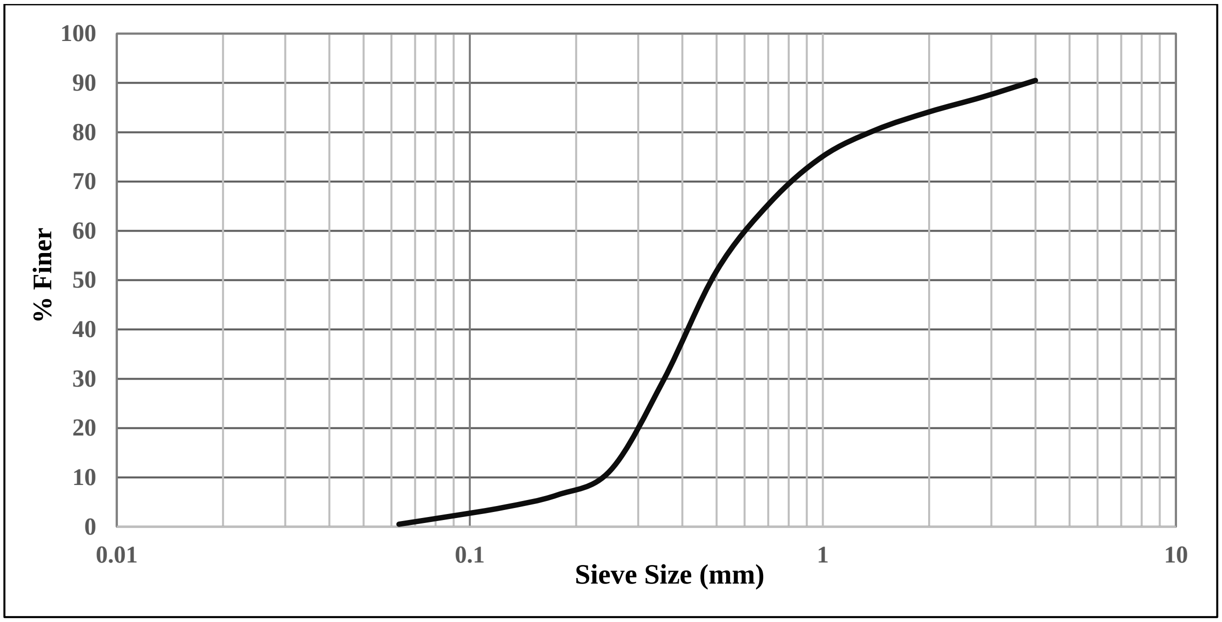


Figure A6. Grain size analysis of the core sample returns 99s2 at a depth of 22.5m, an area at the top of UCCU (Cockfield Formation) presumed to be paleochannel sediments.

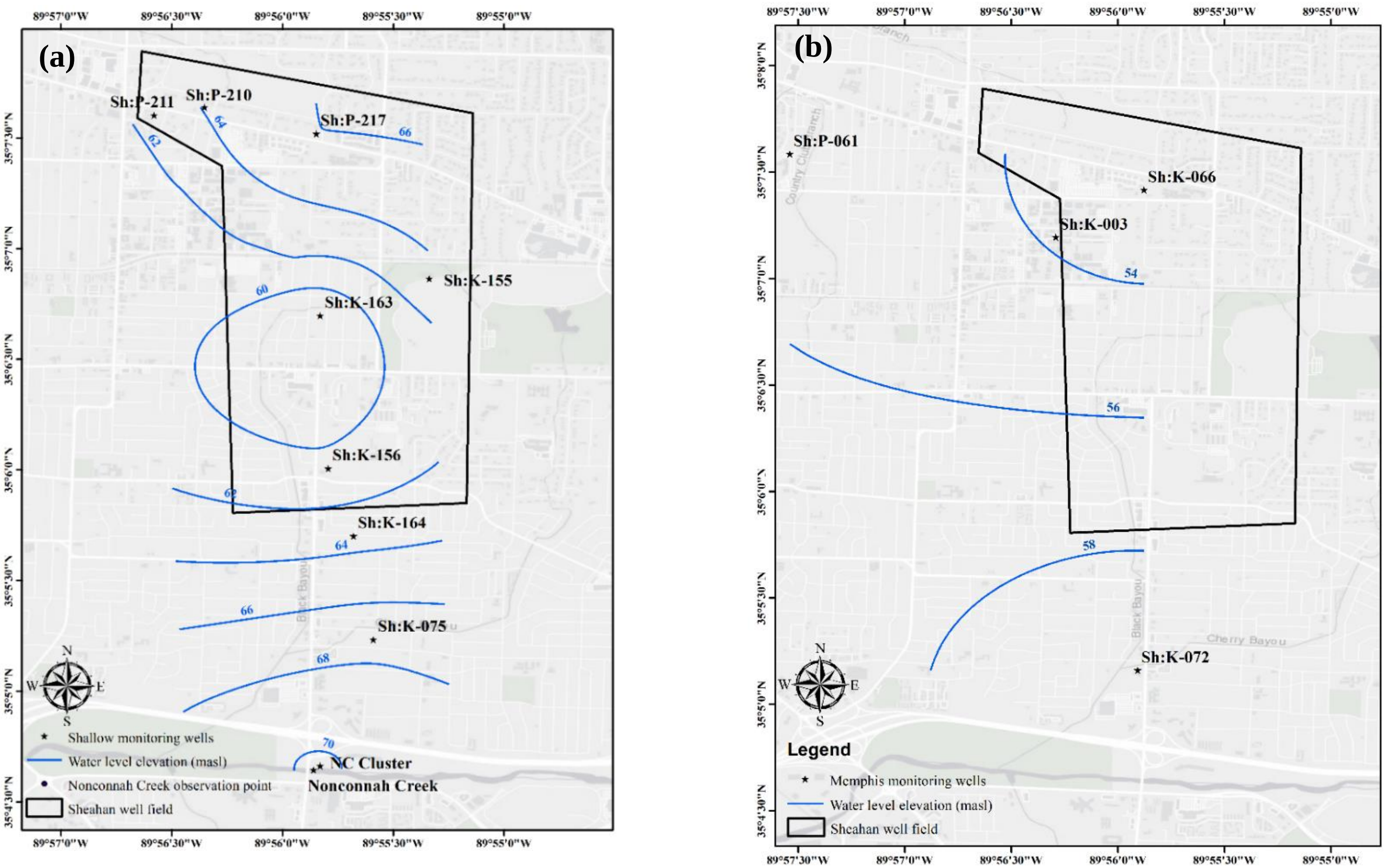


Figure A7. Water level contour map in and around Sheahan well field in July 2020. (a) Water-table surface map (b) Memphis aquifer potentiometric surface map.