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Subject: Calibration of the Transient Coastal Region II SEAWAT Model (Final)

1.0 INTRODUCTION

The Northwest Florida Water Management District (NFWFMD, or “the District”) is updating its existing groundwater flow and transport models to assess the need to develop and establish minimum aquifer levels to manage saltwater intrusion in the Upper Floridan aquifer along the coastal portion of Water Supply Planning Region II (Santa Rosa, Okaloosa, and Walton Counties). Modeling tasks include the following: (1) perform transient calibration of the Region II MODFLOW (“R2MF”) groundwater flow model with updated pumpage and hydrologic data, (2) build and verify a sub-regional, Coastal Region II SEAWAT (“CR2SWT”) model from two existing sub-regional DSTRAM models, (3) calibrate the CR2SWT model with updated pumpage, water level, and water quality data, and (4) perform predictive simulations. Tasks 1 and 2 were completed prior to the work documented herein, which addressed the third task—a transient calibration of the existing CR2SWT model (Tetra Tech, 2020a) with updated pumpage, water level, and water quality data.

The transient R2MF model (Tetra Tech, 2020b) was developed based on an earlier, steady-state MODFLOW model of the Upper and Lower Floridan aquifers in planning Region II (HydroGeoLogic, 2000). The CR2SWT model domain is contained entirely within the R2MF model boundaries (**Figure 1**), covers an area of approximately 3,680 square miles, and encompasses portions of five Florida counties (Santa Rosa, Okaloosa, Walton, Washington, and Bay; **Figure 2**). The CR2SWT model described herein is partly based on two sub-regional models (HydroGeoLogic, 2005 and 2007) developed using the DSTRAM code (HydroGeoLogic, 2008). Tetra Tech (2020a) documents the migration of these models—and all pertinent information contained therein—from DSTRAM to SEAWAT Version 4 (Langevin et al., 2003).

This technical memorandum describes updates—including smoothing of layer elevations, boundary condition refinement, and hydraulic and transport-parameter updates—that were made to the existing (i.e. DSTRAM-based) CR2SWT model to enable transient flow and transport simulations from 1942 through 2015. Datasets provided by the District were implemented as calibration targets during an automated calibration—also documented herein—that relied on several variants of the Parameter Estimation (“PEST”) algorithm (Doherty, 2019).

2.0 MODEL CONFIGURATION

2.1 MODEL STRUCTURE

2.1.1 Simulation Period

The transient R2MF and CR2SWT models both simulate annual transient stress periods during a “post-development” period that follows a much longer “pre-development” period. The pre-development period is represented by one, 100-year transient stress period (without any groundwater extraction or injection) in the R2MF model, whereas pre-development is represented by a separate steady-state flow and transient transport simulation in the CR2SWT model. The final pre-development heads in both models (and final pre-development concentrations in the CR2SWT model) are used as initial conditions for the post-development models.

The R2MF model simulates 74 transient annual stress periods representing years 1942 through 2015. The existing (pre-calibration) DSTRAM-based CR2SWT model simulated 57 transient annual stress periods representing 1942-1998 (Tetra Tech, 2020a). Seventeen (17) additional annual stress periods were added to extend the CR2SWT model’s simulation period through 2015, resulting in a total of 74 transient annual stress periods in the new postdevelopment CR2SWT model.

2.1.2 Model Grid and Layering

The existing CR2SWT model grid consisted of 20 layers, 184 rows, and 334 columns (Tetra Tech, 2020a). Spacing of model rows (1292.71 ft, or 394.02 m) and columns (1292.68 ft, or 394.01 m) was constant throughout the model domain. Row and column spacings from the existing CR2SWT model were retained; however, layer elevations from the existing model were revised to smooth contacts between hydrostratigraphic units. An additional (top) layer was added for consistency with the R2MF model and enabled the direct application of R2MF model-simulated heads as time-varying Constant Head (CHD) boundaries in the updated CR2SWT model. Consequently, the updated CR2SWT model has 21 layers and encompasses six (6) distinct hydrostratigraphic units (from top to bottom; see **Figures 3 and 4**):

- Layer 1 represents the surficial aquifer system (including the sand-and-gravel aquifer, where present) and the Gulf of Mexico and its adjoining bays;
- Layers 2-4 represent the Intermediate Aquifer System (IAS; a regional confining unit);
- Layers 5-9 represent the Upper Floridan aquifer (UFA);
- Layers 10-12 represent the Bucatunna clay confining unit (where present) and the undifferentiated Floridan Aquifer System (FAS) where the Bucatunna clay is absent;
- Layers 13-18 represent the Lower Floridan aquifer (LFA); and
- Layers 19-21 represent the Sub-Floridan aquifer system (SUB).

The original documentation of the DSTRAM models (HydroGeoLogic, 2005; HydroGeoLogic, 2007) and Tetra Tech (2020a) provide more detailed descriptions of model layering, hydrostratigraphy, and the hydrogeologic conceptual model upon which the CR2SWT model is based.

2.1.3 Boundary Conditions

Groundwater head boundary conditions within the updated, 21-layer model were assigned as follows:

- CHD boundaries in all cells of the top and bottom model layers;
- CHD boundaries in all outer (perimeter) cells of the UFA (layers 5-9) and LFA (layers 13-18; **Figure 2**);

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- No flow lateral boundaries for the SAS (layer 1), IAS (layers 2-4), and Bucatunna clay (layers 10-12)
- Rivers in layer 5 representing Holmes Creek and the Choctawhatchee River (**Figure 2**); and
- Pumping and injection wells (**Figure 2**).

Concentration boundary conditions within the updated, 21-layer model were assigned as follows:

- Concentrations were specified for all CHD boundary conditions in the top and bottom model layers, and in all outer (perimeter) cells of layers representing the UFA and LFA
- Zero (advective and dispersive) flux boundary conditions were assigned to the lateral boundaries of the layers representing the SAS, IAS, and Bucatunna clay

Groundwater withdrawals and injections were represented as specified fluxes. SEAWAT automatically removes the appropriate amount of dissolved mass from extraction wells, but requires that the concentrations of any injected water are specified in the Source Sink Mixing (SSM) package. Additional details of model boundary conditions are presented below.

2.1.4 Transport Formulation

The CR2SWT model simulates coupled variable-density groundwater flow and transport. The single simulated “species” on which density depends is the relative seawater concentration, or “relative salinity.” Seawater has a relative salinity equal to 1.0 relative salinity unit (RSU), whereas completely fresh water without any dissolved solids has a concentration of 0.0 RSU. This formulation was used in the existing CR2SWT model (Tetra Tech, 2020a) and was retained because of its intuitiveness and the ease with which relative salinity concentrations can be converted to other species of interest (e.g. total dissolved solids, chloride, etc.) using a single conversion factor.

2.2 MODEL UPDATES

In addition to extending the existing CR2SWT model’s simulation period through 2015 and the inclusion of a new top layer (as noted above), some other updates were made to the model. All such revisions are described below.

2.2.1 Layering

The existing CR2SWT model layering was primarily based on elevations defined in the R2MF model datasets (Tetra Tech, 2020a). The same layer elevations were assigned to all CR2SWT model cells with cell centers in a particular R2MF model cell, which resulted in blocks of adjacent cells with the same top and bottom elevations; see Fig. 6 of Tetra Tech (2020a). Hydrostratigraphic unit (HSU) boundary elevations at R2MF model cell centers were interpolated to create a set of smoother hydrogeologic contacts between HSUs (e.g. **Figures 3 and 4**). The top of layer 1, which represents land surface onshore and sea level offshore, was interpolated to the CR2SWT model grid in a similar manner. The resulting HSUs comprising more than one layer were then subdivided using the same proportional specifications used in developing the existing CR2SWT model layering (Tetra Tech, 2020a).

2.2.2 Pre-Development Duration

The existing CR2SWT model simulated a one million (10^6) day pre-development period using steady-state flow and transient transport (Tetra Tech, 2020a). Pre-calibration testing of the existing CR2SWT model indicated that the pre-development simulation’s duration was not long enough to achieve a state of approximate mass transport equilibrium (i.e. expected pre-development conditions). Therefore, the pre-development stress period length was increased to 2×10^8 days. Additional testing prior to model calibration indicated that 2×10^8 days was a sufficiently

long simulation period to approach approximate mass transport equilibrium¹ (given the pre-calibration aquifer properties and boundary conditions).

2.2.3 Specified Concentrations

The pre-development model's initial concentrations and the boundary concentrations specified for both models (i.e. pre- and post-development) at the top, bottom, and lateral boundaries were all updated prior to calibration.

2.2.3.1 Initial Concentrations

The PEST utility ELEV2CONC1 (Doherty, 2019) was used to estimate initial concentrations for the pre-development model. The inputs and assumptions required to use ELEV2CONC1 were specified based partly on recommendations from District staff and are as follows:

1. Model cell-specific estimates of the elevations at which the relative concentration is equal to 0.5 RSU, or half the salinity of seawater (provided by the District);
2. The vertical width of the freshwater-saltwater interface (3,000 ft, based on a District recommendation);
3. The concentrations assigned to seawater (1.0 RSU, or 35,000 mg/L TDS) and freshwater (0.0025 RSU, or approximately 88 mg/L TDS); and
4. The change in water density per unit change in concentration (1.657 lb/ft³/RSU).

The concentrations generated by ELEV2CONC1 were used as initial conditions for the first pre-development model run. The initial concentrations of subsequent pre-development runs were specified as the final simulated pre-development concentrations from an earlier run; therefore, the ELEV2CONC1 results were only utilized once. This approach of periodically updating the pre-development model's initial conditions resulted in better approximations of pre-development flow and transport conditions during calibration than if the ELEV2CONC1 results—which were farther from a state of mass transport equilibrium—had been used during calibration.

2.2.3.2 Boundary Concentrations

The concentrations generated by ELEV2CONC1 were also used to specify concentrations at the CR2SWT model's bottom and lateral UFA and LFA CHD boundaries. Boundary concentrations were assumed to be constant with time and the concentrations estimated by ELEV2CONC1 were assigned throughout the pre- and post-development models to the CHD boundaries in the sub-Floridan, UFA, and LFA. Water entering the model from the constant head boundaries in layer 1 was assumed to have a concentration of 1.0 RSU at saline boundaries (the Gulf of Mexico and the adjoining bays²; **Figure 5**) and a concentration of 0.001 RSU at freshwater boundaries³.

¹ The pre-development simulation is not intended to represent historic conditions, but rather to achieve an approximate state of mass transport equilibrium suitable for use as initial condition for the calibration period. The length of time required to reach such a state is more reflective of the initial conditions used in the pre-development simulation than the time that was required (historically) to reach an approximate equilibrium state.

² Several pre-calibration simulations were executed to assess the sensitivity of model results to the salinity assigned to the inland bays connected to the Gulf of Mexico, which are presumably brackish. Model results indicated that groundwater heads and concentrations at target locations were insensitive to the concentrations assumed for the bays, at least at the outset of the calibration process.

³ The difference in freshwater concentrations assigned to CHDs in layer 1 (0.001 RSU) and the lateral boundaries (0.0025; based on the minimum ELEVCONC1-based concentrations) arose from differences in observed freshwater concentrations in the surficial aquifer and the Floridan aquifer.

Concentrations assigned to the CHD boundaries for the UFA and LFA in the pre- and postdevelopment models were subsequently refined during the CR2SWT calibration (as described in sections 3 and 4 of this report).

The USGS-developed FloPy package (Bakker et al. 2016) was used to automate creation of the Sink and Source Mixing (SSM) Packages in which boundary concentrations are specified. Additional specifications for the boundary condition concentrations used in the CR2SWT model are provided in the FloPy implementation description (below).

2.2.4 Constant Head Boundaries

Groundwater heads specified for the time-varying CHD boundaries encapsulating the model domain were based on heads simulated by the R2MF model and generated by ELEV2CONC1. In addition to producing initial concentration estimates, ELEV2CONC1 also produces corresponding “zero flow heads” in equilibrium with the estimated concentrations. The constant head values assigned to all cells in the bottom model layer—part of the Sub-Floridan formation, which is not represented in the R2MF model—were equal to the ELEV2CONC1-generated “zero flow heads.” The bottom layer specified heads are assumed to be constant with time and are therefore identical in the pre- and post-development models. Time-varying constant head boundaries in all layer 1 cells (e.g. **Figure 5**) and around the model’s perimeter in the UFA and LFA were assigned head values based on spatial interpolation of the transient heads simulated by the R2MF model to CR2SWT cell centers.

PEST utilities (Doherty, 2019) and FloPy were used to automate extraction of head information from the R2MF model’s outputs and write the pre- and post-development models’ CHD Packages. Additional details concerning CHD boundary specifications are provided in the FloPy implementation description below.

2.2.5 River Boundaries

The RIV Package was used in the existing CR2SWT model to represent the portions of Holmes Creek and the Choctawhatchee River that intersect the UFA (**Figure 2**). However, all sections of Holmes Creek and the Choctawhatchee River were not represented in the RIV Package of this version of the model. As a result, the RIV Package was revised such that both waterbodies were continuous and RIV boundary conductances were representative of the river lengths present in each cell. The RIV conductances were subsequently scaled such that the total conductance of all RIV boundaries matched the base (unscaled) total conductance of UFA RIV cells in the R2MF model. Applying this scaling methodology made the RIV conductance multiplier parameter value from the R2MF model calibration (Tetra Tech, 2020b) directly transferrable to the CR2SWT model.

2.2.6 Groundwater Extraction and Injection Rates

The pumping and injection rates provided by the District and used in the R2MF model (Tetra Tech, 2020b) were the basis for the CR2SWT model pumping and injection rates. Pumping and injection well locations are shown in Figure 2. Due to the finer vertical discretization of the CR2SWT model relative to the R2MF model, pumping and injection rates were redefined using the total rates from the R2MF model and well depth interval information provided by the District. Well depth intervals were analyzed to determine the CR2SWT model layer(s) to which the R2MF model pumping rates should be assigned. In instances where a portion of each pumping well’s open interval intersected a confining unit (based on the CR2SWT model layer elevations), the elevation of the top or bottom of the open interval (as appropriate) was reassigned to the top or bottom elevation of the nearest aquifer layer. Well depth intervals and pumping/injection rates were then imported into Groundwater Vistas (Environmental Simulations, 2017), which was used to produce the post-development model’s Well (WEL) Package based on (1) the intersected layer(s), (2) pumping/injection rates, and (3) pre-calibration aquifer conductivities from the calibrated R2MF model.

2.3 PROCESSING FRAMEWORK

Existing PEST-compatible pre- and post-processing utility programs were used to automate all necessary model pre-processing and post-processing steps. Pre-processing utilities were employed to create the inputs necessary to execute the CR2SWT model, and post-processing utilities were used to extract (and convert, if necessary) model-generated outputs to be compared with calibration targets.

2.3.1 Pre-Processing

2.3.1.1 Transient R2MF Model Simulation and Post-Processing

The entire pre-processing, model execution, and post-processing framework used during calibration of the R2MF model (Tetra Tech, 2020b) was embedded within the CR2SWT model calibration process (**Figure 6**). That is, each time the CR2SWT model was executed the R2MF model was also run using the same, updated values for shared parameters between the two models (e.g. conductivity pilot point values inside the CR2SWT model domain). This “nesting” of the R2MF model within the CR2SWT model pre-processing was desirable to maintain conceptual consistency between the CR2SWT model’s parameters and parameters from the larger model upon which most of its CHD boundary conditions are based.

After execution of the complete R2MF model processing framework, the PEST suite utility MOD2OBS1 was used to spatially and temporally interpolate the R2MF model-simulated heads to estimate heads at CR2SWT model cell centers in layer 1, the UFA, and LFA. The resulting heads were used to generate CHD boundary conditions for the CR2SWT model simulations. Heads from the end of the R2MF model’s first (i.e. pre-development) stress period were assigned to the pre-development CR2SWT model, and R2MF model-simulated heads at the beginning and end of each annual stress period were assigned to the beginning and end of the corresponding CR2SWT model post-development stress periods.

2.3.1.2 FloPy Script Processing

A script written in the Python programming language (version 3.7; van Rossum and Drake, 2009) that invoked the FloPy Package was used to generate pre- and post-development CHD Packages (**Figure 6**). All data inputs, including the temporally varying R2MF model-simulated heads at CR2SWT model nodes (i.e. MOD2OBS1 outputs), were read into Python using the PANDAS open-source library (McKinney, 2020).

Heads simulated by the R2MF model in the surficial aquifer (R2MF model layer 1) were assigned to the CHD boundaries in layer 1 of the CR2SWT model. Layer 1 R2MF model cells with simulated heads below the bottom of layer 1 (“dry cells”) were assigned CHD boundary heads equal to the given cells’ bottom elevation plus 0.1 ft. Lateral CHD boundaries in the UFA and LFA (CRSWT layers 5-9 and 13-18, respectively) were assigned R2MF model-based heads from corresponding cells along the perimeter of the UFA and LFA layers (R2MF model layers 3 and 5, respectively). The bottom CR2SWT model CHD boundaries were assigned the “zero flow heads” generated by ELEV2CONC1 (Doherty, 2019).

The “CHDDENSOPT” option in SEAWAT Version 4 was invoked for both the pre- and post-development simulations (Langevin et al., 2003). All layer 1 CHD boundaries were assigned a CHDDENSOPT value of 1, which allows the user to assign cell-specific densities to be used in converting the specified (point-water⁴) CHD heads to the

⁴ Point-water head is based on the density at the point where head is measured, or “head in terms of the native aquifer water” (Langevin et al., 2003).

reference (equivalent freshwater⁵) heads used internally by SEAWAT. Layer 1 densities were assigned based on location; onshore cells were uniformly assigned a density of 62.442 (lb/ft³) to represent freshwater and cells in the Gulf of Mexico and adjoining bays were assigned a density of 64.001 (lb/ft³) to represent saline water (1.0 RSU).

Lateral and bottom CHD boundaries were not assigned CHDDENSOPT values of 1, and therefore did not require specified densities. Lateral boundaries were assigned a CHDDENSOPT value of 3, which results in SEAWAT interpreting the specified lateral boundary heads as reference (or, equivalent freshwater) heads. To be consistent with the “zero flow heads” produced by ELEV2CONC1, the layer 21 CHD boundaries were assigned a CHDDENSOPT value of 2, which instructs SEAWAT to interpret the specified layer 21 heads as environmental heads⁶.

2.3.1.3 Boundary Concentrations

Concentrations for all sources of water are specified in the Source-Sink Mixing (SSM) Packages. All layer 1 constant head boundaries were specified as constant concentration cells (ITYPE = -1). As with the specified heads, the assigned layer 1 constant concentrations were based on location (**Figure 5**): onshore cells were assigned a groundwater concentration of 0.001 RSU (35 mg/L TDS) and cells representing the Gulf of Mexico and adjoining bays were assigned concentrations of 1.0 RSU (35,000 mg/L TDS). The sub-Floridan (layer 21) CHD cells were also assumed to be constant concentration cells, and the concentrations were assumed to be equal to those produced by ELEV2CONC1 throughout the entire simulation period.

To allow simulated concentrations to vary around the edges of the Upper and Lower Floridan Aquifers, the lateral CHD boundaries were not treated as constant concentration cells but were instead identified only as CHD boundaries in the SSM Package (i.e. ITYPE = 1). Concentrations for the lateral UFA and LFA CHD boundaries were initially assigned based on ELEV2CONC1 outputs. During the calibration process it became apparent that these concentrations were adversely impacting the ability to match the lowest concentration calibration targets. As a result, a set of 100 (50 UFA and 50 LFA) lateral boundary concentration scaling (LBCS) parameters were introduced to allow PEST to adjust the lateral boundary concentrations generated by ELEV2CONC1. Each LBCS parameter represents a coefficient by which the ELEV2CONC1-based concentration at a given point (**Figure 7**) was multiplied to produce the concentration specified in the CR2SWT models. Values at LBCS points were linearly interpolated to determine scaling values in model cells between points. Coinciding UFA and LFA points in the undifferentiated FAS were assigned the same multiplier value to ensure increasing salinity with increasing depth.

The concentration of any water entering the model from the RIV boundaries representing Holmes Creek and the Choctawhatchee River was assumed to be 0.001 RSU (35 mg/L TDS). The concentrations of injected water from two LFA injection wells (NWF_3770 and NWF_7911) were also specified in the SSM Package (**Figure 6**) and were based on historic injection well concentration data provided by the District.

⁵ Density is assumed to be temperature-independent and a function of only one dissolved species (“relative salinity” per Section 2.1.4). Therefore, the reference heads used in the solution of the variable-density flow equations are “equivalent freshwater heads,” or the height of a hypothetical column of freshwater, and represent the potential for horizontal flow. When two points at the same elevation but different horizontal locations in the groundwater flow system have identical equivalent freshwater heads, no horizontal flow between these two points will occur.

⁶ Environmental head is the water level of a hypothetical well filled with water that has a vertical concentration distribution of salinity identical to that of the surrounding column of groundwater. Environmental head represents the potential for vertical flow. Where two vertically-separated (but horizontally-coincident) points in the groundwater flow system have identical environmental heads, then there should be no vertical flow between these two points,

2.3.1.4 Hydraulic Property Kriging and Interpolation

The spacing and locations of pilot points used to represent the model's various hydraulic properties were selected during calibration of the R2MF model (Tetra Tech, 2020b). Kv pilot points in layers 10-12 are irregularly spaced (**Figure 8**) to allow for greater refinement of the transition from the Bucatunna clay-confined portion of the LFA to the undifferentiated FAS. Pilot point locations are regularly spaced (**Figure 9**) for all other properties represented using pilot points. The PLPROC utility (Doherty, 2016) was used to krig and interpolate smooth parameter fields for all pilot point-based properties:

1. Kv of the IAS and SUB;
2. Kh of the UFA and LFA; and
3. Kv, Kh/Kv, and specific storage of the BUC/undifferentiated FAS layers.

2.3.1.5 Parameter Translations

The PAR2PAR utility (Doherty, 2019) was used to perform the following functions:

1. Scale river boundary conductance values using the riverbed conductance multiplier and write the MODFLOW River Package,
2. Facilitate the conversion of undifferentiated FAS Kh pilot point values to Kv pilot point values using the undifferentiated FAS Kh/Kv, and
3. Assign and populate the layer 10-12 storage pilot point file with Bucatunna clay or UFA storage values (as appropriate)⁷.

The TWOARRAY utility (Doherty, 2019) was used to calculate the necessary Kh arrays for the IAS, SUB, BUC/undifferentiated FAS layers from (1) the vertical hydraulic conductivity arrays written by PLPROC and (2) each group of layers' respective horizontal-to-vertical hydraulic conductivity anisotropies (Kh/Kv).

2.3.2 Post-Processing

After each CR2SWT model simulation was completed, six (6) post-processing utilities from the PEST suite were used to extract model results for comparison to calibration targets: BUD2SMP1, MOD2OBS1, MOD2SMPDIFF, OBS2OBS, SMP2SMP, and SMPDIFF (Doherty, 2019). Further details concerning the calibration targets identified in this section can be found in Section 3.1.

The MOD2OBS1 utility was used to spatially and temporally interpolate simulated groundwater heads and concentrations from output times and locations to target times and locations. OBS2OBS was then used to calculate (1) composite simulated concentrations at target wells open to multiple layers and, subsequently, (2) simulated temporal and vertical concentration differences at target wells. The MOD2SMPDIFF and SMP2SMP utilities were used to extract simulated vertical and horizontal head differences, whereas SMP2SMP and SMPDIFF were used to determine simulated temporal head differences. Simulated incremental changes in baseflows were calculated using the BUD2SMP1 utility and were temporally interpolated to estimate flows at target dates—June 30 of each year—using SMP2SMP.

⁷ Properties at pilot points where the Bucatunna clay is absent in the eastern portion of layers 10-12 were assigned the same values as the LFA (layers 13-18).

3.0 MODEL CALIBRATION

3.1 CALIBRATION TARGETS

Transient calibration of the updated CR2SWT model was performed in order to satisfactorily replicate observed groundwater heads, groundwater salinities, and spatiotemporal differences in heads and salinities during the post-development period (1942-2015). As in the transient R2MF model calibration (Tetra Tech, 2020b), simulated post-development changes in river baseflows were also monitored and used as qualitative (i.e. non-quantitative) calibration targets during the CR2SWT model calibration. Groundwater head and concentration target locations are summarized in Appendix Table A-1.

3.1.1 Groundwater Heads

A subset of the groundwater head measurements provided by the District for the transient R2MF model calibration (Tetra Tech, 2020b) were used to inform and guide the CR2SWT model calibration process. The resulting mean annual head target dataset included 78 well locations (**Figure 10**) and 1,666 head targets (**Appendix Table A-2**). For practical purposes, mean annual groundwater head measurements were assumed to represent conditions at the approximate midpoint of each year (June 30) during calibration.

The R2MF model head targets were assigned to the CR2SWT model layer containing the well midpoint (based on open interval information provided by the District). If the resulting CR2SWT model layer was not in the same HSU as the R2MF model target, the head target was assigned to the nearest CR2SWT model layer in the same HSU; for instance, if the open interval midpoint of a well was in layer 4 (IAS) but the target was treated as a UFA target during the R2MF model calibration, the CR2SWT model target was reassigned to the uppermost UFA layer (i.e. layer 5).

3.1.2 Head Differences

Head difference target datasets from the R2MF model calibration were also used as CR2SWT model calibration targets (**Appendix A**). The individual wells used to develop head difference targets for the R2MF model were chosen to capture the observation-based shape and timing of development of the extraction-induced cone of depression in the UFA. All R2MF model vertical and horizontal head difference targets (VHDs and HHDs, respectively) from well pairs inside the CR2SWT model domain were used in the CR2SWT model calibration, as were all R2MF model temporal head difference (THD) targets from wells inside the CR2SWT model domain.

A total of two (2) vertical well pairs from the R2MF calibration dataset were retained (**Appendix Table A-3; Figure 11**). Both well pairs included one UFA and one LFA well and provided a total of 40 vertical head difference targets.

Horizontal head difference (HHD) targets were based on concurrent differences between mean annual groundwater heads at a well located near the center of the UFA cone of depression (NWF ID = 1894 in the UFA and NWF ID = 3210 in the LFA; **Figure 12**) and mean annual groundwater heads from wells in the same HSU surrounding the center well. A total of nine (9) well pairs were identified—seven (7) in the UFA and two (2) in the LFA—which provided a total of 387 horizontal head difference targets (**Appendix Table A-4**).

Temporal head difference (THD) targets were created to ensure the calibrated model would be able to capture the timing of the cone of depression development at individual wells. Wells with longer records of measurements were chosen for THDs, and individual head difference targets were calculated as the difference between each head measurement and the latest (i.e. most recent) reliable head measurement. Altogether 26 wells were chosen (**Figure 13**) and 926 temporal head difference targets were defined for these wells (**Appendix Table A-5**).

3.1.3 Baseflow Targets

Upstream-to-downstream differences in baseflow within the SEAWAT domain were calculated using the final calibration R2MF model (Tetra Tech, 2020b). These baseflow difference targets were assigned weights of zero, and therefore did not contribute to the objective function being optimized, but were periodically compared to cumulative simulated River Package flows to ensure the CR2SWT model results did not deviate substantially from the R2MF model results (which simulated baseflows acceptably; Tetra Tech, 2020b). Baseflow difference targets are provided in **Appendix Table A-6**.

3.1.4 Concentration Targets

Annual summary statistics for specific conductance (SC), total dissolved solids (TDS), chloride (Cl) concentrations, and sodium (Na) concentrations were provided by the District to be used in developing annual concentration targets. All four types of data were not available for every target location during every year of record. Therefore, in order to utilize as much data as possible and maximize the number of calibration targets, a hierarchical approach was used to convert the annual median concentration data to relative salinity targets:

1. For locations and years with TDS measurements, TDS was converted to relative salinity using a conversion factor ($35,000 \text{ mg/L TDS} = 1.0 \text{ RSU}$; Sverdrup et al., 2000) and used as the relative salinity target for that well and year.
2. At locations and during years without any TDS measurements, the relative salinity target was based on SC measurement data (if available) and was calculated using a conversion factor⁸ of $66,400 \text{ }\mu\text{S/cm} = 1.0 \text{ RSU}$.
3. When TDS and SC data were unavailable, Na concentrations were used to calculate targets (if available) and were converted to relative salinity targets using a conversion factor of $10,800 \text{ mg/L Na} = 1.0 \text{ RSU}$ (Turekian, 1968).
4. When only Cl measurements were provided, Cl was converted to a relative salinity target using a conversion factor of $19,400 \text{ mg/L Cl} = 1.0 \text{ RSU}$ (Turekian, 1968).

The relative salinity targets developed based on this hierarchy were reviewed by Tetra Tech and District staff. Individual targets that either appeared to be erroneous (e.g. based on earlier and/or later concentrations trends) or were based on one or more questionable measurements were assigned weights of zero during calibration. The resulting concentration target dataset consisted of 107 locations (**Figure 14**) with a total of 1,581 non-zero weighted targets (**Appendix Table A-7**). The final calibration target dataset consisted of 1,434 targets (approximately 91%) based on TDS measurements, 130 (approximately 8%) based on SC measurements, 17 (approximately 1%) based on Na measurements, and none (zero) based on Cl measurements.

An abrupt horizontal concentration gradient developed along the model's southern boundary during the calibration process. This gradient led to numerical instabilities in the flow and transport solution during some calibration runs and, consequently, hindered the automated calibration process. Synthetic (estimated) offshore concentration calibration targets (**Appendix Table A-8**) were added for layers 7 (UFA) and 15 (LFA) at the locations shown in **Figure 7** to encourage PEST to eliminate this sharp concentration gradient and the resulting instabilities.

3.1.5 Concentration Differences

The concentration target dataset was used to develop vertical concentration difference (VCD) and temporal concentration difference (TCD) targets. A total of seven (7) well pairs (**Figure 15**) were determined to be suitable

⁸ This conversion factor is based on a linear regression between TDS and SC in the concentration target dataset.

locations for VCD estimates and were used to define 50 targets (**Appendix Table A-9**). Thirty-three (33) wells (**Figure 16**), including all 25 wells with significant ($p < 0.05$) temporal concentration trends, were used to develop 548 TCD targets (**Appendix Table A-10**).

3.1.6 Target Groups and Weighting

A calibration plan was developed prior to calibration that included a description of how the initial target datasets would be subdivided into groups and subsequently weighted during calibration. The District-approved calibration plan is reproduced in **Appendix B**.⁹ Per this calibration plan, targets were subdivided into 12 groups: seven (7) head-based groups and five (5) concentration-based groups. Head targets were subdivided into four time periods: 1942-1965, 1966-1990, 1991-2000, 2001-2015. Concentration targets were subdivided into three groups based on the target value: 0-150 mg/L Cl (or equivalent), 150-350 mg/L Cl (or equivalent), and greater than 350 mg/L Cl (or equivalent). The three head difference target types (VHDs, HHDs, and THDs) and two concentration difference target types (VCDs and TCDs) were each assigned to a separate target group which, when combined with the four head target groups and three concentration target groups, accounted for all 12 target groups.

Prior to calibration, each target group was reweighted using the PWTADJ1 utility (Doherty, 2019) to ensure that each group of targets contributed equally to the objective function (“Phi”) value at the outset of the calibration process. Weights were subsequently refined during calibration by emphasizing certain target groups in order to improve calibration metrics.

3.2 CALIBRATION PARAMETERS

A total of 499 calibration parameters were adjusted during the automated calibration. Most of these parameters—398, or approximately 80% of all adjustable calibration parameters—represented horizontal or vertical hydraulic conductivities at pilot points (**Figures 8 and 9**)¹⁰. As in the R2MF model calibration (Tetra Tech, 2020b), the surficial aquifer (Layer 1) was assumed to have a uniform horizontal hydraulic conductivity (K_h), which was not modified during calibration. All other hydrostratigraphic units were assigned spatially variable hydraulic conductivities using pilot points. The calibration parameters that were not hydraulic conductivity pilot points were:

1. HSU-specific values of horizontal-to-vertical anisotropy (K_h/K_v ; 6 calibration parameters);
2. HSU-specific values of storage coefficient for the IAS, UFA, BUC, LFA, and SUB (5 calibration parameters);
3. Longitudinal dispersivity (α_L) for layers 1-4 (1 calibration parameter);
4. HSU-specific longitudinal dispersivities for the UFA, BUC, LFA, and SUB (4 calibration parameters);
5. Porosity of layers 1-4 (1 calibration parameter);
6. HSU-specific porosities of the UFA, BUC, LFA, and SUB (4 calibration parameters);
7. Lateral boundary concentration scaling parameters (79 calibration parameters); and
8. A domain-wide scaling factor (multiplier) applied to the base RIV conductance values (1 calibration parameter).

Pilot points were used to spatially interpolate layer 10-12 storage coefficients, however the 103 pilot points used for this purpose (**Figure 9**) were assigned one of two values: pilot points in areas where the Bucatunna clay was present (i.e. red pilot point locations in **Figure 8**) were assigned the Bucatunna clay’s storage coefficient, and pilot

⁹ Note: A revised concentration dataset was provided by the District after the Calibration Plan was finalized, which led to the differences in target numbers between the Calibration Plan and Appendix A.

¹⁰ Only pilot points located inside the CR2SWT model domain were adjusted during calibration.

points in areas where the Bucatunna clay was absent (i.e. the yellow pilot point locations in **Figure 8**) were assigned the LFA storage coefficient.

The pilot point-based calibration parameters consisted of:

1. Unique vertical hydraulic conductivity (K_v) pilot points encompassing all of the IAS (77 pilot points) and SUB (77 pilot points; **Figure 9**),
2. Unique horizontal hydraulic conductivity (K_h) pilot points encompassing all of the UFA (77 pilot points) and LFA (77 pilot points; **Figure 9**), and
3. Unique vertical hydraulic conductivity (K_v) pilot points encompassing the western and southern portions of layers 10-12 (which represents the Bucatunna clay) and the Bucatunna clay-to-undifferentiated Floridan Aquifer System (FAS) transition (64 pilot points; red and green locations, respectively, in **Figure 8**). The 40 undifferentiated FAS pilot points in layers 10-12 (yellow locations in **Figure 8**) were assigned K_v values based on the K_h of the coinciding LFA pilot point and the LFA horizontal-to-vertical anisotropy ratio (K_h/K_v), which resulted in layer 10-12 K_h values that were nearly identical to those in the LFA where the Bucatunna clay formation is absent.

3.2.1 Initial Values and Ranges

Initial calibration parameter estimates and allowable ranges for flow parameters common to both the R2MF and CR2SWT models were based on the final calibrated R2MF parameter values (Tetra Tech, 2020b). Parameters shared by both models included conductivities at pilot points, HSU-specific anisotropies, HSU-specific storage parameters, and the RIV boundary conductance multiplier.

When incorporated into the calibration process, all LBCS factors were assigned initial values of 1.0 and were allowed to vary between 0.01 and 1.0 during the calibration process. Initial values for the remaining parameter values—dispersivities and porosities—were based on the existing CR2SWT model, which had a domain-wide longitudinal dispersivity of 100 ft and domain-wide porosity of 0.25. Several sensitivity simulations were executed before calibration, which revealed that a longitudinal dispersivity of 10 ft resulted in a better match to the concentration target dataset than did a 100 ft value; as a result, the 10 ft longitudinal dispersivity was assigned to all model layers at the calibration outset. The allowable ranges for dispersivity and porosity were 1-100 ft and 0.05-0.30, respectively. The ratios between (i) longitudinal and horizontal transverse dispersivity (α_{TH}/α_L) and (ii) longitudinal and vertical transverse dispersivity (α_{TV}/α_L) were prespecified (fixed) as 0.2 and 0.01, respectively.

3.3 CALIBRATION METHODS

Two variants of the PEST software suite (Doherty, 2019) were used during calibration of the CR2SWT model: PEST_HP (Doherty, 2020) and PEST++ (Welter et al., 2012). Each variant was selected to take advantage of the different strengths of each variant during the calibration process. Calibration runs executed during the calibration process are documented in **Appendix C**.

Additional simulations were executed after the automated calibration process was concluded. The goal of these simulations was to determine the effects of specific changes to certain parameter values on calibration metrics. These simulations included decreasing the SUB's specific storage (from 1E-03 to 1E-04 ft⁻¹) and modifying the values of three offshore LBCS parameter values to be better aligned with nearby LBCS parameters. Upon analysis of the results of these simulations, the only changes included in the final calibration model were the three offshore LBCS parameter revisions.

4.0 CALIBRATION RESULTS

The calibration metric goals defined before the calibration process (“Goals”) and the corresponding calibration metric values for the calibrated CR2SWT model are presented in **Table 1**.

4.1 CALIBRATION PARAMETERS

Calibration parameter naming conventions are summarized in **Table 2**. Parameter bounds and the final (calibrated) values for all pilot point-based hydraulic conductivity parameters and LBCS parameters are provided in **Appendix D**. The parameter bounds and final values for all non-pilot point calibration parameters are provided in **Table 3**.

Calibrated horizontal hydraulic conductivities of the UFA and LFA are illustrated in **Figures 17 and 18**, respectively. Corresponding transmissivities of all UFA layers (5-9) and LFA layers (13-18) were calculated from these horizontal hydraulic conductivities and are shown in **Figures 19 and 20**. Calibrated vertical hydraulic conductivities of the IAS and layers 10-12 are illustrated in **Figures 21 and 22**, respectively. The resulting leakances of the IAS and layers 10-12 are illustrated in **Figures 23 and 24**, respectively. The storage coefficient of cells in layers 10-12 were calculated by first assigning the storage coefficient value of the Bucatunna clay or that of the LFA (as appropriate) to each of the 103 pilot points shown in **Figure 9**, and subsequently interpolating from the pilot point locations to the model grid. The resulting distribution is shown in **Figure 25**.

4.2 CALIBRATION TARGETS

All calibration targets and corresponding simulated values are provided in **Appendix A**. Calibration target and target group naming conventions are summarized in **Tables 4a and 4b**, respectively. Observed and simulated well hydrographs and concentration time-series at target locations are presented in **Appendix E**.

4.2.1 Head Targets

Mean and mean absolute head residuals for each target well during the model simulation period are illustrated in **Figures 26 and 27**, respectively. Observed and simulated head values for the entire target dataset are compared in **Figure 28**. Observed UFA contours (provided by the District) and simulated head contours in layer 7 (i.e. the middle layer of the UFA) are shown for 2000 and 2015 conditions in **Figures 29 and 30**. The heads simulated in layer 15 (LFA) for 2015 conditions are shown in **Figure 31**. The mean absolute errors for all VHD targets are shown in **Figure 32**, and the individual target and simulated VHD targets are compared in **Figure 33**. Mean absolute errors of HHD targets are shown in **Figure 34** and a comparison of target and simulated HHD targets is shown **Figure 35**. THD mean absolute errors are shown in **Figure 36**, and a comparison of the target and simulated THD targets is shown in **Figure 37**.

4.2.2 Concentration Targets

The RSU concentrations simulated by the model and all target concentrations, concentration differences, and concentration metrics were converted from RSU to TDS for reporting purposes (per the District’s request) using the conversion factor noted above (i.e. 1.0 RSU = 35,000 mg/L TDS).

Mean and mean absolute residuals for each concentration target well during the post-development simulation period are illustrated in **Figures 38 and 39**. The entire concentration target dataset and simulated equivalent concentrations are compared in **Figure 40**. Simulated concentrations at the end of the post-development simulation (2015) are shown in **Figures 41 and 42** for layers 7 (UFA) and 15 (LFA). Mean absolute errors of VCD targets are shown in **Figure 43**, and the individual target and simulated VCD targets are compared in **Figure 44**. TCD mean absolute errors are shown in **Figure 45**, and a comparison of the individual target and simulated TCD targets is shown in **Figure 46**.

4.3 WATER BUDGETS & FLUXES

Domain-wide water budget components from the end of the pre-development simulation, 2000, and 2015 are summarized and contrasted in **Table 5**. Pre-development, 2000, and 2015 rates of leakage from layer 4 (IAS) to layer 5 (UFA) are shown in **Figures 47, 48, and 49**, respectively. Positive values in **Figures 47-49** indicate downward flow from the IAS to the UFA (i.e. UFA recharge) and negative values indicate upward flow.

4.4 MASS BUDGETS

Model domain-wide mass budgets from the end of the pre-development simulation, 2000, and 2015 are provided in **Table 6**.

5.0 DISCUSSION

5.1 CALIBRATION METRIC GOALS

The CR2SWT model's ability to replicate field observations could not be known prior to the calibration process. Despite this uncertainty, however, all but one of the predefined target metric goals were achieved by the final calibrated model (**Table 1**). The one target metric goal that was not met—the mean absolute error (MAE) goal for groundwater heads (5 ft)—was also not achieved during the R2MF model calibration (Tetra Tech, 2020b). Despite not achieving this aggressive head target goal, the calibrated CR2SWT model meets the 5%-or-less “MAE ÷ Range” goal that is frequently applied as a measure of calibration quality; the CR2SWT model's “MAE ÷ Range” is less than 3% (head target range = 209.5 ft; head MAE = 6.25 ft, **Table 1**). All other target metrics were achieved.

5.2 CALIBRATED PARAMETERS

5.2.1 Flow Parameters

The final values of flow-related calibration parameters not defined using pilot points (**Table 3**) reveal several patterns. The CR2SWT calibration process resulted in further refinements to the R2MF model's horizontal-to-vertical anisotropy estimates. Model-wide anisotropy (K_h/K_v) in the IAS increased from a midrange value in the R2MF model calibration (32.0) to the upper bound of 52.5, whereas K_h/K_v in the Bucatunna clay/undifferentiated FAS was modified only minimally (from 36.9 in the R2MF model calibration to 33.2; **Table 3**). The anisotropy of the UFA layers was reduced from 2.04 in the R2MF model to 1.0. The LFA anisotropy increased from 17.9 initially to the maximum bound (52.5). The specific storage of the UFA and LFA layers decreased to the minimum values assigned during calibration, whereas the SUB specific storage increased to the maximum allowable value. The calibrated IAS and BUC/undifferentiated FAS specific storage values were similar ($4.4E-04$ and $1.3E-04$ ft⁻¹, respectively) and fell between the minimum and maximum bounds. The specific yield of the surficial aquifer is not used because this layer consists entirely of constant head cells.

Hydraulic conductivities in the five HSUs with spatially varying (i.e. pilot point-based) conductivities generally followed one of two patterns: widespread changes or subtle, localized refinements to the initial R2MF model-based conductivities. Widespread increases in the vertical hydraulic conductivity of the SUB occurred during the CR2SWT calibration process; K_v at 95 of the 103 SUB K_v pilot points (“kv6” pilot points in **Appendix D**) increased during calibration with a mean increase of 363% over the initial (DSTRAM-based) values. The calibration process decreased K_v at 69 of 77 IAS pilot points with a mean decrease of 53% from the initial (R2MF-based) values. K_v in the IAS (**Figure 21**) exhibits a clear increasing trend from northwest-to-southeast.

Hydraulic conductivities in all the other HSUs (UFA, BUC, LFA) underwent more localized modifications during calibration. As in the R2MF model calibration results, the only clear spatial pattern in UFA and LFA conductivities

and transmissivities is an area of higher values in the east-central portion of the model domain (**Figures 17-20**), which is consistent with the available APT estimates. The Bucatunna clay-to-undifferentiated FAS transition in layers 10-12 is reflected by the relatively sharp transition in leakance over a relatively short horizontal distance (**Figure 24**). This sharp transition from the undifferentiated FAS to where the LFA is confined by the Bucatunna clay is consistent with the conceptual model and was present in the original (HydroGeoLogic, 2000) and updated R2MF models (Tetra Tech, 2020b).

5.2.2 Solute Transport Parameters

Transport-related calibration parameters were varied by HSU (**Table 3**). The initial porosities of the six HSUs (all of which were 0.25 based on the original CR2SWT model; Tetra Tech, 2020a) were increased during calibration such that the separately calibrated porosities of all HSUs were all equal to the maximum allowable value (0.30; **Table 3**). The initial dispersivity value assigned to all HSUs (10 ft) was increased in the surficial aquifer, IAS, LFA and SUB layers. Calibrated dispersivity values in these layers range from 45-70 ft, whereas the most optimal dispersivities of the UFA and BUC/undifferentiated FAS layers were identified as being the lowest allowable value (1 ft).

5.3 WATER BUDGETS & FLUXES

The instantaneous domain-wide water budgets from the end of the pre-development model, 2000, and 2015 reveal several noteworthy patterns (**Table 5**). The lateral UFA CHD boundaries are the single most dominant source of water (i.e. inflow) to the model during each of the three selected periods. Nearly half of the simulated inflow ($8.34\text{E}+06$ out of $1.72\text{E}+07$ ft³/d, or 49%) during pre-development comes from lateral UFA CHDs, which remain high through the end of the post-development period. The dominance of lateral flow in the UFA is to be expected considering the large contrast between K_h in the UFA layers (**Figure 17**) and K_v in the over- and underlying HSUs (**Figures 21 and 22**). The other most significant inflows originate from the LFA lateral CHDs (27-30% of inflows), river inflows (9-12%), and the layer 1 CHDs (12-13%). Inflows from wells and storage are generally low during the two selected post-development periods, although inflows from storage in 2000 (which was a drought year) comprise more than 9% of the total model inflows ($1.77\text{E}+06$ out of $1.87\text{E}+07$ ft³/d).

The greatest outflow during all three periods is to the rivers in layer 5. During pre-development, river outflows comprise nearly 82% of the total outflow. River outflows in 2000 and 2015 comprise less of the total model outflow (62% and 64%, respectively) than during pre-development due to increases in other outflows (e.g. pumping) and small reductions in river outflow rates with time. Groundwater pumping constitutes the second greatest outflow during both 2000 ($4.64\text{E}+06$ ft³/d, or 21% of the total outflow) and 2015 ($3.52\text{E}+06$ ft³/d, or 17% of the total outflow). Outflows to the LFA lateral CHDs range from 5-6% of the total outflows. UFA lateral CHD outflows are in the 6-8% range, and all other outflows are generally in the 0-2% range.

The reduction in outflows to the layer 1 CHDs from pre-development through 2015 (**Table 5**) is clear when comparing the magnitude and direction of leakage between the IAS and UFA in pre-development, 2000, and 2015 (**Figures 47-49**). The red areas in **Figure 47** indicate widespread upward flow under pre-development conditions, whereas reductions in UFA head (resulting from groundwater pumping) induced downward flow by 2000 which persisted through 2015. As simulated by the R2MF model (Tetra Tech, 2020b), the reductions in pumping in coastal Bay County between 2000 and 2015 resulted in the reestablishment of an upward hydraulic gradient by 2015 in this area (**Figures 48 and 49**).

5.4 MASS BUDGETS

Boundary mass fluxes are the products of boundary concentrations and volumetric boundary flows. Mass budgets therefore tend to be dominated by boundary flow rates in areas with high boundary concentrations. This can lead to seemingly counterintuitive model results, particularly when boundary concentrations vary over several orders of

magnitude (e.g. 0.001 to 1.0 RSU) as in the CR2SWT model. Nevertheless, mass budgets can still provide some useful insights when this limitation is understood.

Mass flux rates at the end of pre-development, 2000, and 2015 (**Table 6**) all indicate that constant head boundaries are the greatest mass source to the model domain. Rivers are the greatest mass sink at all three times. The magnitude of net mass losses to rivers decreases over the course of the simulation due to both reductions in outflow and increases in inflows. Mass injected via groundwater injections is minimal in 2000 and 2015 (0.32% and 0.15% of mass inflows, respectively). Groundwater pumping removes approximately 21% of all extracted mass in 2000 and 16.5% of all removed mass in 2015.

Initiation of groundwater pumping and injection resulted in a 3.7% reduction in mass inflow from constant heads between pre-development and 2000 (i.e. $3.6\text{E}+07$ mass units per day). Conversely, reductions in pumping rates from 2000 to 2015 (**Table 5**) resulted in a 6.3% ($5.9\text{E}+07$ mass units per day) increase in constant head boundary mass inflow (by $5.8\text{E}+07$ mass units per day). The relative magnitude of these mass inflow rate differences is small and—since boundary concentrations are constant with time—can be attributed to relatively small differences in the magnitudes of inflow rates across constant head boundaries between the three time periods.

5.5 CALIBRATION TARGETS

5.5.1 Groundwater Heads

The calibrated CR2SWT model shows minimal bias in simulated post-development groundwater heads (mean error, “ME” = 0.78 ft; **Table 1**). Examination of the ME and MAE results by target well for the entire simulation period also indicate minimal spatial bias. Wells with positive and negative errors are interspersed (**Figure 26**) and wells with larger MEs and MAEs are interspersed with wells with lower errors (**Figures 26 and 27**). Head targets near the eastern model boundary are primarily in the Upper Floridan layers and tend to be underestimated (**Figure 26**); however there are also several UFA wells in this area that are overestimated.

There is also minimal temporal bias in the head target results. Mean head errors during the 1942-1965, 1966-1990, 1991-2000, and 2001-2015 periods (i.e. “head_grp1” through “head_grp4”) are -0.57 ft, 1.90 ft, 0.81 ft, and -2.54, respectively. The slightly degradation in mean error from the 1991-2000 period to the 2001-2015 period is at least partly attributable to targets at new observation wells installed after 2000 in which heads were typically underestimated but temporal head trends were reproduced well by the model. Mean absolute head errors during these same time periods are 5.85 ft, 5.78 ft, 6.40 ft, and 6.49, respectively. Relatively small temporal differences in mean absolute error indicate that the calibration model replicates groundwater heads equally well throughout the simulation period.

5.5.2 Head Differences

Observed vertical head differences are reproduced well by the model based on the VHD “MAE ÷ Range” metric (3.62%; **Table 1**). The overall direction and magnitude of the vertical head gradients are simulated accurately for those targets with more than a 10 ft head difference (**Figure 33**). Horizontal head differences between the well pairs shown in **Figure 12** are simulated very well based on the observed versus simulated comparison (**Figure 35**) and the “MAE ÷ Range” metric (6.81%; **Table 1**). Inspection of mean absolute errors of the individual HHD target well pairs (**Figure 34**) reveals that the range in UFA HHD well pair MAEs is approximately 7-12 ft, and that the two LFA HHD well pair MAEs range from approximately 4-7 ft. The model’s proven ability to replicate observed vertical and horizontal head differences during the calibration period suggest the model is a suitable tool for predicting the magnitude and direction of saltwater movement in the future.

THDs are also generally replicated well, as indicated by the THD “MAE ÷ Range” metric (5.62%; **Table 1**). The greatest THD mean absolute errors are near the center of the pumping-induced cone of depression in southern Okaloosa County (**Figure 36**). This apparent spatial bias is not unexpected, or necessarily indicative of a poorly

calibrated model, given that the temporal head differences of the greatest magnitudes were observed in this area (see well hydrographs in **Appendix E**). There appears to be an overestimation bias in the CR2SWT model's THD targets (**Figure 37**), and no such bias was apparent in the final calibrated R2MF model (Tetra Tech, 2020b).

5.5.3 Groundwater Concentrations

As was the case with the head target dataset, there is minimal bias in simulated groundwater salinities ($ME = 0.0010$ RSU = 35 mg/L TDS; **Table 1**). There does not appear to be a spatial bias in concentration errors in either the UFA or LFA considering that positive and negative residuals (**Figure 38**) and larger and smaller magnitude residuals (**Figure 39**) are interspersed. The model tends to underestimate concentration targets greater than 1000 mg/L TDS (**Figure 40**), including the LFA targets in Santa Rosa County (**Figure 38**). However, the lower range of observed concentrations (i.e. <1000 mg/L TDS)—which notably includes the TDS secondary Maximum Contaminant Level (500 mg/L) and from a management perspective is the more important concentration range to match—is neither systematically overestimated or underestimated.

5.5.4 Concentration Differences

Although all concentration difference targets meet their respective metric goals (**Table 1**), concentration difference targets are generally not matched as well as head difference targets. For example, the VCDs in five of the seven VCD well pairs are replicated quite well (**Figures 43 and 44**), but the other two VCD pairs have target values in the 2800-4500 mg/L TDS range (**Figure 44**) and residuals of approximately 1500 and 4000 mg/L TDS (**Figure 43**). There is also substantial scatter about the perfect fit line for the TCD targets (**Figure 46**), but the overall trend of temporal differences simulated where temporal differences are observed is replicated by the model.

5.5.5 Baseflow Targets

The qualitative incremental baseflow targets are matched well (**Appendix A**). All baseflow target values (range: 165-175 ft³/s, “cfs”) are higher than the simulated values (range: 129-145 cfs), and the average error is 19% (range: 18-22%). Although all annual baseflow targets are underestimated, it should be noted that these targets are based entirely on results from the calibrated R2MF model and are, therefore, uncertain.

The reduction in (net) simulated baseflow discharge between the two models occurred despite the increase in riverbed conductance multiplier from 6.29 (R2MF model; Tetra Tech, 2020b) to 10.0 (**Table 3**). The increased baseflow discharge that this increase in conductance would suggest was evidently offset by the recalibrated UFA properties and lower simulated layer 5 heads relative to the UFA layer in the R2MF model (layer 3).

6.0 CONCLUSIONS

The CR2SWT model was calibrated to replicate mean annual groundwater levels, groundwater salinities, and spatiotemporal differences in groundwater levels and salinity. The final calibration model generated acceptable error metrics with respect to these calibration targets during the calibration period (1942-2015). Now that the CR2SWT model has been calibrated, it is well-suited to predict the impacts of various sets of potential future conditions (e.g. pumping regimes) on the movement of water and salt mass in the Floridan Aquifer System within Water Supply Planning Region II.

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