A Salinity Module for SWAT to Simulate Salt Ion Fate and Transport 1 at the Watershed Scale 2 3

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10 Abstract. Salinity is one of the most common water quality threats in river basins and irrigated regions worldwide. However, no 11 available numerical models simulate all major processes affecting salt ion fate and transport at the watershed scale. This study 12 presents a new salinity module for the SWAT model that simulates the fate and transport of 8 major salt ions ($SO_4^{2^-}$, Ca^{2^+} , Mg^{2^+} , 13 Na⁺, K⁺, Cl⁻, CO₃²⁻, HCO₃⁻) in a watershed system. The module accounts for salt transport in surface runoff, soil percolation, 14 lateral flow, groundwater, and streams, and equilibrium chemistry reactions in soil layers and the aquifer. The module consists of 15 several new subroutines that are imbedded within the SWAT modelling code and one input file containing soil salinity and 16 aquifer salinity data for the watershed. The model is applied to a 732 km² salinity-impaired irrigated region within the Arkansas 17 River Valley in southeastern Colorado, and tested against root zone soil salinity, groundwater salt ion concentration, 18 groundwater salt loadings to the river network, and in-stream salt ion concentration. The model can be a useful tool in simulating 19 baseline salinity transport and investigating salinity best management practices in watersheds of varying spatial scales.

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21 **1** Introduction

22 Salinity is one of the most common water quality threats in river basins and irrigated regions worldwide. Sustainability of 23 crop production in irrigated areas in semi-arid and arid areas is threatened by over-irrigation, poor quality of irrigation water 24 (high salinity), inadequate drainage, shallow saline groundwater, and salinization of soil and underlying groundwater, all of 25 which can lead to decreasing crop yield. Of the estimated 260 million ha of irrigated land worldwide, approximately 20-30 26 million ha (7-12%) is salinized (Tanji and Kielen, 2002), with a loss of 0.25 to 0.5 million ha each year globally. Approximately 27 8.8 million ha in western Australia alone may be lost to production by the year 2050 (NLWRA, 2001), and 25% of the Indus 28 River basin is affected by high salinity. Within the western United States, 27-28% of irrigated land has experienced sharp 29 declines in crop productivity due to high salinity (Umali, 1993; Tanji and Kielen, 2002), thereby rendering irrigated-induced 30 salinity as the principal water quality problem in the semi-arid regions of the western United States.

31 Salinization of soil and groundwater systems is caused by both natural processes and human-made activities. Salt naturally 32 can be dissolved from parent rock and soil material, with salt minerals (e.g. gypsum CaSO4, halite NaCl) dissolving to mobile 33 ions such as Ca²⁺, SO₄²⁻, Na⁺, and Cl⁻. In addition, salt ions can accumulate in the shallow soil zone due to waterlogging, which is 34 a result of over-irrigating and irrigating in areas with inadequate drainage. Salts moving up into the soil zone can become evapo-35 concentrated due to the removal of pure water by crop roots. Soil water salinization leads to a decrease in osmotic potential, i.e. 36 the potential for water to move from soil to the crop root cells via osmosis, leading to a decrease in crop production.

37 Numerical models have been used extensively to assess saline conditions, simulate salt movement across landscapes and 38 within soil profiles, predict salt build-up and movement in the root zone, and investigate the impact of best management 39 practices (Oosterbaan, 2005; Schoups et al., 2005; Burkhalter and Gates, 2006; Singh and Panda, 2012). Available models that 40 either have inherent salinity modules or can be applied to salinity transport problems include UNSATCHEM (Šimunek and

- 41 Suarez, 1994), HYDRUS linked with UNSATCHEM (Šimůnek et al., 2012); DRAINMOD, LEACHC (Wagenet and Hutson,
- 42 1987), SAHYSMOD (Oosterbaan, 2005; Singh and Panda, 2012), CATSALT, and MT3DMS (Burkhalter and Gates, 2006).
- 43 Whereas several of these models include major ion chemistry for salt ions (e.g. precipitation-dissolution, cation exchange, 44 complexation) (UNSATCHEM, HYDRUS), their application typically is limited to small field-scale or soil-profile domains (e.g. 45 Kaledhonkar and Keshari, 2006; Schoups et al., 2006; Kaledhonkar et al., 2012; Rasouli et al., 2013). Conversely, models such 46 as SAHYSMOD and MT3DMS have been applied to regional-scale problems, but lack the reaction chemistry and treat salinity 47 as a conservative solute. SAHYSMOD uses seasonal water and salt balance components for large-scale systems on a seasonal 48 time step (Singh and Panda, 2012). MT3DMS is a finite-difference contaminant transport groundwater model that uses 49 MODFLOW output for groundwater flow rates, but does not include salt ion solution chemistry (Burkhalter and Gates, 2006). 50 Schoups et al. (2005) used a hydro-salinity model that couples MODHMS with UNSATCHEM to simulate subsurface salt 51 transport and storage in a 1400 km² region of the San Joaquin Valley, California. The model, however, does not consider salinity 52 transport in surface runoff or salt transport in streams, limiting results to soil salinity and groundwater. Currently, there is no 53 model that simulates salt transport in all major hydrologic pathways (surface runoff, soil percolation and leaching, groundwater 54 flow, streamflow) at the watershed-scale that also considers important solution reaction chemistry. Such a model is important for 55 assessing watershed-scale and basin-scale salt movement and investigating the impact of large-scale salinity remediation 56 schemes.
- 57 The objective of this paper is to present a salinity transport modeling code that can be used to simulate the fate and transport of the major ions (SO₄²⁻, Ca²⁺, Mg²⁺, Na⁺, K⁺, Cl⁻, CO₃²⁻, HCO₃⁻) in a watershed hydrologic system. The salinity module is 58 59 implemented within the SWAT modeling code, and thereby salt transport pathways include surface runoff, percolation, soil 60 lateral flow, groundwater flow and streamflow. The soil water and groundwater concentration of each salt ion is also affected by 61 equilibrium chemistry reactions: precipitation-dissolution, complexation, and cation exchange. The use of the model is 62 demonstrated through application to a 732 km² region of the Lower Arkansas River Valley (LARV) in southeastern Colorado, an 63 irrigated alluvial valley in which soil and groundwater salinization has occurred over the past few decades. The model is tested 64 against salt ion and total dissolved solids (TDS) concentration in surface water (Arkansas River and its tributaries), groundwater 65 (from a network of monitoring wells), and soil water (from a large dataset of soil salinity measurements). The salinity module for 66 SWAT can be applied to any watershed to simulate baseline conditions and to test the effect of best management practices on 67 watershed salinity.
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69 2 Development of the SWAT Salinity Module

This section provides a brief overview of the SWAT model, followed by a description of the SWAT salinity module. Sect. 3 demonstrates the use of the salinity module to a regional-scale irrigated stream-aquifer system in the Lowe Arkansas River Valley, Colorado.

73 2.1 The SWAT Model

The SWAT (Soil and Water Assessment Tool, Arnold et al., 1998) hydrologic model simulates water flow, nutrient mass transport and sediment mass transport at the watershed scale. It is a continuous, daily time-step, basin-scale, distributedparameter watershed model that simulates water flow and nutrient (nitrogen, phosphorus) transport in surface runoff, soil percolation, soil lateral flow, groundwater flow and discharge to streams, and streamflow. The watershed is divided into subbasins, which are then further divided into multiple unique combinations (Hydrologic Response Units HRUs) of land use, soil type and topographic slope for which detailed water and nutrient mass balance calculations are performed. Routing algorithms route water and nutrient mass through the stream network to the watershed outlet. SWAT has been applied to hundreds of 81 watersheds and river basins worldwide to assess water supply and nutrient contamination under baseline conditions (Abbaspour 82 et al., 2015) and scenarios of land use change (Zhao et al., 2016; Zuo et al., 2016; Napoli et al., 2017), best management 83 practices (Arabi et al., 2006; Maringanti et al., 2009; Ullrich and Volk, 2009; Dechmi and Skhiri, 2013), and climate change 84 (Jyrkama and Sykes, 2007; Ficklin et al., 2009; Tweed et al., 2009; Haddeland et al., 2010; Brown et al., 2015). However, it has 85 not yet been applied to salinity issues.

86 2.2 Salinity Module for SWAT

The new SWAT salinity module allows SWAT to simulate the fate and transport of 8 major salt ions $(SO_4^{2-}, Ca^{2+}, Mg^{2+}, Na^+, K^+, Cl^-, CO_3^{2-}, HCO_3^{-})$ via surface runoff, soil lateral flow, soil percolation and leaching, groundwater flow, and streamflow, subject to chemical reactions such as precipitation-dissolution, complexation, and cation exchange within soil layers and the alluvial aquifer. The module also simulates the loading of salt mass to the soil profile via saline irrigation water from both surface water (subbasin channel) and groundwater (aquifer) sources. A watershed cross-section schematic describing these processes is shown in Figure 1.

93 The salinity module is implemented directly into the SWAT modelling code (FORTRAN), with new subroutines developed 94 for salt chemistry (salt chem), salt irrigation loading (salt irrig), salinity percolation and leaching (salt lch), and salt 95 groundwater transport and loading to streams (salt gw). Other standard SWAT subroutines are modified to incorporate salt ion 96 transport and effects, such as lagging solutes in surface runoff and groundwater flow (surfstor, substor), and routing solutes 97 through the stream network (watqual). These subroutines are shown in Figure 2 within the general SWAT modeling code data 98 flow. For each day loop, the mass balance calculations for each HRU are performed. Salt subroutines are shown for chemical 99 equilibrium, irrigation loading, salt leaching, soil salinity stress, salt groundwater transport and loading, and lagging in surface 100 runoff and groundwater flow. At the end of the HRU calculations, the water, sediment, nutrients, and salt ion mass is routed 101 through the stream network, with in-stream concentration of each salt ion simulated for each SWAT subbasin. Details for each 102 salt ion process are now presented. For the equations presented, S refers to salt mass, and the subscript i refers to the 8 major 103 ions. For the transport equations, calculations are similar to SWAT's transport equations for nitrate. Salinity module input data 104 and output data also will be discussed later in this section.

105 **2.2.1** Salt in Surface Runoff (*"salt_lch"* and *"surfstor"* subroutines)

106 The mass of each salt ion can be transferred from an HRU to the subbasin channel via surface runoff. The salt ion mass 107 generated in surface runoff $S'_{i surf}$ (kg/ha) for the current day is calculated as:

$$108 \qquad S'_{i,surf} = \beta_{S_i} \cdot C_{S_i} \cdot Q_{surf} \qquad (1)$$

109 where β_{S_i} is the salinity percolation coefficient, C_{S_i} is the concentration of the *i*th salt ion in the mobile water for the top 10 mm 110 of soil (kg salt /mm water), and Q_{surf} is the surface water generated from the HRU on a given day (mm water). As only a portion 111 of the surface runoff and lateral flow reaches the subbasin channel on the day it is generated, SWAT uses a storage feature to 112 surface runoff. The salt ion mass reaching the subbasin channel on the current day via surface runoff is calculated as:

113
$$S_{i,surf} = \left(S_{i,surf} + S_{i,surfstor}\right) \cdot \left(1 - \exp\left[\frac{-surlag}{t_{conc}}\right]\right)$$
(2)

114 where $S_{i,surf}$ is the mass of the *i*th salt ion that reaches the subbasin channel on the current day (kg/ha), $S_{i,surfstor}$ is the salt ion 115 surface runoff stored or lagged from the previous day (kg/ha), *surlag* is the surface runoff lag coefficient, and t_{conc} is the time of 116 concentration for the HRU (hrs).

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119 2.2.2 Salt in Lateral Flow ("salt_lch" and "substor" subroutines)

120 The salt ion mass generated in lateral flow $S'_{i lat lv}$ (kg/ha) from a soil layer for the current day is calculated as:

121
$$S'_{i,lat,ly} = C_{S_i} \cdot Q_{lat,ly}$$
 (3)

where $Q_{lat,ly}$ is the water discharge from the layer by lateral flow (mm water). Similar to surface runoff, only a portion of the lateral flow will reach the subbasin channel on the day it is generated, and thus the salt ion mass reaching the channel on the current day $S_{i,lot,ly}$ (kg/ha) via lateral flow is calculated as:

125
$$S_{i,lat,ly} = \left(S_{i,lat,ly} + S_{i,latstor}\right) \cdot \left(1 - \exp\left[\frac{-1}{TT_{lat}}\right]\right) \quad (4)$$

126 where $S_{i,latstor}$ is the salt ion mass stored or lagged from the previous day (kg/ha) and TT_{lat} is the lateral flow travel time (days).

127 **2.2.3** Salt in Soil Percolation (*"salt_lch"* subroutine)

- 128 The salinity module tracks the mass of each salt ion (kg/ha) in each soil layer. The salt ion mass moved to the underlying 129 soil layer by percolation $S_{i, perc, lv}$ (kg/ha) is calculated as:
- 130 $S_{i,perc,ly} = C_{S_i} \cdot Q_{perc,ly}$ (5)

where $Q_{perc,ly}$ is the amount of water percolating to the underlying soil layer on a given day (mm water). After percolation has been simulated, the concentration of each salt ion (mg/L) in each soil layer is calculated using the area (m²) of the HRU and the volume of water in the soil layer (m³). The leached salt ion mass is added to the shallow aquifer using the following:

134
$$S_{i,rech} = \left[\left(1 - g w_{delay} \right) \cdot S_{i,perc} \right] + \left(g w_{delay} \cdot S_{i,rech,t-1} \right)$$
(6)

135 where $S_{i,rech}$ is the salt ion mass loaded to the water table via recharge (kg/ha), $S_{i,perc}$ is the salt ion mass percolated from the

bottom layer of the soil profile, $S_{i,rech,t-1}$ is the leached salt ion mass from the previous day, and gw_{delay} is the groundwater delay

137 time, i.e. the time required for water leaving the bottom of the root zone to reach the water table (days).

138 **2.2.4 Salt in Groundwater Flow (***"salt_gw"* subroutine)

139 The salinity module tracks the mass of each salt ion (kg/ha) in the aquifer. The salt ion mass generated in groundwater flow 140 $S'_{i,m}$ (kg/ha) from the aquifer for the current day is calculated as:

141
$$S'_{i,gw} = C_{S_{i,gw}} \cdot Q_{gw}$$
 (7)

142 where $C_{S_{i,gw}}$ is the salt ion concentration in the aquifer (kg salt /mm water), and Q_{gw} is the groundwater flow generated for the HRU

for the current day (mm water). The concentration of each salt ion in each HRU aquifer is calculated on each day by dividing the
total mass of the salt ion (g) by the total volume of groundwater (m³).

145 2.2.5 Salt in Streamflow (*"watqual"* subroutine)

Water is routed through the watershed channel network using the variable storage routing method, a variation of the kinematic wave model (Neitsch et al., 2011). The mass of each salt ion is routed through the channel network with water, with no chemical reactions changing in-stream salt ion concentration. Similar to any constituent in SWAT, salt ion loadings (kg/day) can be specified for any subbasin reach of the watershed.

150 **2.2.6** Salt in Irrigation water (*"salt_irrig"* subroutine)

151 Salt ion mass is added to the soil profile via irrigation water, with water derived from either the aquifer (groundwater 152 pumping) or from surface water diversions. Including constituent mass in irrigation water is a new feature for SWAT, as the original code does not account for nutrient (N, P) mass in irrigation water. If the irrigation water source is a subbasin reach (surface water irrigation), the concentration of each salt ion is multiplied by the volume of applied irrigation water (depth of water * HRU area) to determine the mass of each salt ion (kg/ha) to add to the first soil layer. If the irrigation water source is the shallow aquifer, the concentration of each salt ion in the HRU aquifer is used to estimate salt loading to the first soil layer. The salt ion mass is then removed from the HRU aquifer.

158 2.2.7 Salt Solution Chemistry

The salinity chemistry implemented into SWAT is based on the Salinity Equilibrium Chemistry (SEC) module developed for soil-aquifer systems (Tavakoli-Kivi et al., 2019). The equations for salinity solution chemistry presented here are performed for each HRU soil layer and for each HRU. The solution chemistry in this module is similar to that implemented in other water chemistry models [UNSATCHEM: Šimůnek et al. (2012), PHREEQC: Parkhurst and Appelo (2013), MINTEQA2: Paz-Garcia et al. (2013)]. Thus, only basic details are presented here.

The SEC module includes 8 aqueous components, 10 complexed species, five solid (salt mineral) species, and four exchange species (Table 1). The 8 aqueous components $(SO_4^{2-}, Ca^{2+}, Mg^{2+}, Na^+, K^+, C\Gamma, CO_3^{2-}, HCO_3^{-})$ are included due to their presence in the majority of soil-aquifer systems. The five salt minerals (CaSO₄, CaCO₃, MgCO₃, NaCl, MgSO₄) also are included due to their presence in many soil-aquifer systems, although the module can be amended to include any mineral species. The module simulates the dissolved concentration (mg/L) of the 8 ions in soil water and groundwater and the solid mass concentration of the five salt mineral species in the soil and the aquifer sediment according to precipitation-dissolution, complexation, and cation exchange reactions.

For these calculations, the duration of the model time step (daily time step for SWAT) is assumed long enough for all constituent reactions to achieve equilibrium. The concentration of species at equilibrium is calculated using a stoichiometric algorithm approach, in which mass balance and mass action equations are solved simultaneously. This method is used in other water chemical equilibrium packages such as PHREEQC (Parkhurst and Appelo, 2013) and MINTEQA2 (Paz-Garcia et al., 2013).

176 Law of Mass Action

177 At equilibrium, the concentration of all reactants and products are related using the equilibrium constant *K*:

178
$$K = \frac{(C)^{c} (D)^{d}}{(A)^{a} (B)^{b}}$$
 (8)

where A and B are reactants, C and D are products, *a*, *b*, *c*, and *d* are constants, and the parentheses denote solute activities. The activity of the *i*th solute, *i*_A, is computed by multiplying the activity coefficient γ_i by the molal concentration, where γ_i depends on the ionic strength *I* of the solution:

182
$$I = \frac{1}{2} \sum m_i z_i^2$$
 (9)

183 where z_i is the charge number of the i^{th} ion and m_i is the molality (mol/kg H₂0). γ_i is then given as:

184
$$\begin{cases} \log \gamma_{i} = -\frac{A_{a}z_{i}^{2}\sqrt{I}}{1+B_{a}a_{i}\sqrt{I}} & I < 0.1\\ \log \gamma_{i} = -Az_{i}^{2}\left(\frac{\sqrt{I}}{1+\sqrt{I}} - 0.3I\right) & 0.1 < I < 0.5 \end{cases}$$
(10)

185 where A_a and B_a are temperature dependent constants ($A_a = 0.5085 \text{ m}^{-1}$ and $B_a = 0.3285 \times 10^{10} \text{ m}^{-1}$ at 25° C) and a_i is a measure of

186 effective diameter of a hydrated ion *i*. The first equation in (10) is the Debye-Huckle equation for dilute solutions, and the second

187 equation is the Davis equation.

188 Mass Balance Equations

189 The mass of each element in the system, either in ion or complexed form, is tracked by a set of mass balance equations.

190 Equations for SO₄, Cl, Ca, and Na are:

- 191 $SO_{4_{\tau}} = [SO_4^{2_{\tau}}] + [CaSO_4^{0_{\tau}}] + [MgSO_4^{0_{\tau}}] + [NaSO_4^{1_{\tau}}] + [KSO_4^{1_{\tau}}]$ (11a)
- 192 $Cl_{T} = [Cl^{-}]$ (11b)
- 193 $Ca_{T} = [Ca^{2^{+}}] + [CaSO_{4}^{0}] + [CaCO_{3}^{0}] + [CaHCO_{3}^{+}]$ (11c)
- 194 $Na_{T} = [Na^{+}] + [NaSO_{4}^{+}] + [NaCO_{3}^{0}] + [NaHCO_{3}^{0}]$ (11d)
- where *T* denotes total concentration and brackets indicate species' molality. Similar equations are written for Mg, K, CO₃, andHCO₃.
- 197 Precipitation-Dissolution Reactions
- 198 Salt minerals (AB_s) can dissolve or precipitate according to the stoichiometric reaction
- 199 $AB_s \leftrightarrow A^+_{aq} + B^-_{aq}$ (12)
- 200 The salt mineral will dissolve if the solution is under-saturated in regards to A^{+}_{aq} and B^{-}_{aq} , and will precipitate if the solution is
- super-saturated. Salt minerals in the SEC module include CaSO₄, CaCO₃, MgCO₃, MgSO₄, and NaCl, due to their common occurrence in aquifers. For example:

203
$$CaSO_4 \leftrightarrow Ca^{2+} + SO_4^{2-}$$
 (13)

with a solubility product constant:

205
$$K_{sp_{CaSO_4}} = \frac{(Ca^{2+})(SO_4^{2-})}{(CaSO_4)}$$
 (14)

Within the SEC module, minerals are added to the system one at a time, with the solubility limits of each mineral used to determine the direction of each reaction (precipitation or dissolution).

- 208 Complexation Reactions
- Based on the law of mass action, equilibrium equations are written for all complexed species. For example, the equation for $CaSO_{4}^{0}$ is:

211
$$K_{CaSO_4} = \frac{(Ca^{2+})(SO_4^{2-})}{CaSO_4^0}$$
 (15)

212 where K_{CaSO_4} is the equilibrium constant and is equal to 0.004866. Equations and equilibrium constants for the remaining 9

- 213 complexed species are shown in Supporting Material.
- 214 Cation Exchange Reactions

215 Cation exchange is calculated to determine the sorbed and released ions from sediment surfaces to the solution. The order of 216 replaceability is Na > K > Mg > Ca, determined by Coulomb's Law. The cation reaction as an equivalent reactions represented 217 by Gapon equation:

- 218 $X_{1/mM} + 1/n N^{n+} = X_{1/nN} + 1/m X^{m+}$ (16)
- 219 where $X_{1/mM}$ is exchangeable cation M on the surface (meq/100g), $X_{1/nN}$ is exchangeable cation N on the surface (meq/100g), M
- and N are metal cations, and m + and n + are the charges of cations M and N respectively. Using the cation exchange capacity of

- the soil and a coefficient of Gapon selectivity coefficient for each reaction, concentration of each exchangeable species is determined.
- The salinity chemistry reactions (precipitation-dissolution, complexation, cation exchange) are simulated for each HRU within the *salt_chem* subroutine (see Figure 2). Within this subroutine, the chemistry reactions are applied to the current simulated concentration values of the 5 salt minerals and the 8 salt ions for each soil layer and aquifer, to calculate new concentration values. These new concentration values are then used to simulate salt leaching (*salt_lch* subroutine) and salt ion loading in surface runoff (*surfstor*) and groundwater flow (*salt_gw*, *substor*) (Figure 2). At the end of each daily time step, the simulated salt ion mass (kg) in each transport pathway (irrigation, leaching, runoff, percolation, lateral flow, groundwater flow, dissolution/precipitation) is stored for mass balance assessment and output.

230 2.2.8 Salinity Module Input/Output

- Required data for running the SWAT salinity module include: precipitation-dissolution solubility products for the five salt minerals (CaSO₄, CaCO₃, MgCO₃, NaCl, MgSO₄), initial concentration of salt ions in soil water and groundwater, and initial salt mineral solid concentration (% of bulk soil) in soil and aquifer sediment. Initial concentrations are required for each HRU. However, as will be shown in Sect. 3.3.2.4, using uniform (i.e. each HRU given the same value) concentration values yields the same result as using spatially-variable initial concentrations, if a warm-up period of several years is used in the SWAT simulation.
- All input data are provided in the file "*salt_input*". To turn on the salinity module, a single line has been added to the end of the *file.cio* file, with a flag (0 or 1) being read to exclude/include the salinity module. If the flag is set to 1, the SWAT code will open and read the contents of the *salt_input* file.
- Four output files contain simulated salt ion data for the watershed (Figure 2):
- *salt.output.std* contains the total salt mass (TDS) transported via lateral flow, groundwater flow, surface runoff, tile
 drains, percolation, irrigation of surface water, irrigation of groundwater, upflux water, and dissolution, normalized
 to the area of the watershed (kg/ha).
- *salt.output.rch* contains loading (kg) and concentration (mg/L) of each salt ion for each subbasin channel, for each day of the simulation. Results from this file can be used to plot time series of salt ion concentration, as shown in Sections 3.3.2.1.
- *salt.output.sub* contains the total salt mass (TDS) transported via lateral flow, groundwater flow, surface runoff, tile
 drains, percolation, irrigation of surface water, irrigation of groundwater, and dissolution for each subbasin, for
 each day of the simulation. The salt loads (kg/ha) are normalized to the subbasin area.
- *salt.output.hru* contains salt ion concentration in the soil water and in the groundwater for each HRU, for days
 specified in the *salt_input* file.
- 252

253 3 Application of SWAT Salinity Module to an Irrigated Stream-Aquifer System

254 3.1 Study Region: Lower Arkansas River Valley, Colorado

The salinity module is tested for a 732 km² irrigated stream-aquifer system along the Arkansas River in southeastern Colorado (Figure 3A). The region consists the Arkansas River and tributaries (e.g. Timpas Creek, Crooked Arroyo, see Figure 3A) running through and over a thin (~10-15 km in width) and shallow (~10-20 m) sandy alluvial aquifer. The climate is semiarid, requiring irrigation to supplement rainfall for crop growth. Irrigation water is derived either from the Arkansas River via a

- system of irrigation canals or from the aquifer via a network of ~500 pumping wells (Figure 3A). Cultivation and associated
- 260 irrigation occurs March through November.
- Salinization of soil, groundwater, and surface water in the region has steadily worsened since the 1970s due to increased irrigation diversions from the Arkansas River, high water tables due to excessive water applications to fields, and the existence of salt minerals, particularly gypsum (CaSO₄) (Konikow and Person, 1985; Goff et al., 1998; Gates et al., 2002; Gates et al., 2016). Soil salinity levels under about 70% of the area exceed threshold tolerance for crops, with the regional average of crop yield reduction from salinity and waterlogging estimated to range from 11 to 19% (Gates et al., 2002; Morway and Gates, 2012).
- 266 From sampling groundwater from a network of 82 observation wells (see Figure 3B) (sampling from June 2006 to May 267 2010), average salinity concentration of shallow groundwater is approximately 2700 to 3000 mg/L, and annual salt loading to the 268 Arkansas River from groundwater return flows is about 500 kg per irrigated ha, per km of the river. In the 1990s, 68% of 269 producers stated that high salinity levels are a significant concern (Fraser et al., 1999). For the region modeled in this study, 270 average TDS concentration (C_{TDS}) in groundwater is 3334 mg/L (443 samples), with a minimum of 459 mg/L and a maximum of 271 44600 mg/L. The presence of gypsum is revealed in the high concentration of SO₄ (C_{SO4}), with average, minimum, and 272 maximum concentrations of 1878 mg/L, 147 mg/L, and 29457 mg/L, respectively. Average soil water salinity, based on 273 electrical conductivity of a soil paste extract (EC_e), is 4.11 dS/m (54700 measurements), with minimum and maximum of 0.9 274 dS/m and 56.5 dS/m, respectively (Morway and Gates, 2012). These values were estimated from measurements of apparent bulk 275 soil conductivity, taken with a Geonics EM-38 electromagnetic induction sensor, as described in Morway and Gates (2012). 276 Surveys were performed during the months of March-September for 1999-2005. Based on 6 surface water sampling sites (4 in 277 the Arkansas River, 2 in tributaries; Figure 3B), average C_{TDS} and C_{SO} is 1145 mg/L and 560 mg/L, respectively. More details of
- 278 observed groundwater, soil water, and surface water concentrations are provided in Sect. 3.3.2 when model results are presented.

279 3.2 SWAT Model

280 A previously calibrated and tested SWAT model for the study region is used to simulate salt fate and transport using the 281 developed salinity module. The SWAT model is detailed in Wei et al. (2018). The region was divided into 72 subbasins (see 282 Figure 3B). The digital elevation model (DEM), stream network, soil map, land-use map, climate data, streamflow, and canal 283 diversion data were obtained from the USGS, NRCS, and several state agencies, as summarized in Wei et al. (2018). A method 284 was developed to apply SWAT to highly-managed irrigated watersheds, and included: designating each cultivated field as an 285 individual HRU (see Figure 3B for the map of fields); crop rotations to simulate the effects of changing crop types for each field 286 during the 11-year simulation; seepage to the aquifer from the earthen irrigation canals; and SWAT's auto-irrigation algorithms 287 to trigger irrigation events based on plant water demand for both surface water irrigation and groundwater irrigation. The method 288 resulted in 5270 HRUs. Implementing canal seepage required a slight change to the SWAT modeling code to add pre-processed, 289 estimated canal seepage to the HRU aquifer. Canal seepage rates were obtained from field measurements (Susfalk et al., 2008; 290 Martin et al., 2014).

The model was run for the 1999-2009 time period, with simulated streamflow compared to observed hydrographs at 5 stream gages (Rocky Ford, La Junta, Las Animas, Timpas Creek, Crooked Arroyo; see Figure 3B) for model testing (Wei et al., 2018). Calibration was performed using SWAT-CUP (Abbaspour et al., 2008) using the observed streamflow at the Rocky Ford, Las Animas, and Timpas Creek stations. Twenty parameters were targeted for modification during the calibration process, with the following exhibiting strong control on streamflow: SCS runoff curve number, Manning's *n* value for the main channel, effective hydraulic conductivity of the channel, initial volume of groundwater, recharge delay time, fraction of deep aquifer 297 percolation, and snowfall temperature. Further details regarding calibration, model implementation, and hydrologic results are

298 found in Wei et al. (2018).

299 3.3 SWAT Model with Salinity Module

300 3.3.1 Model Construction and Simulation

The SWAT model with the new salinity module is run from April 1 1999 to December 13 2009, with observed data for testing available from June 2006 to December 2009. The 1999-2005 period thus serves as a warm-up simulation period. The calibration period is 2006-2007, and the testing period from 2008-2009. Required inputs include initial soil water and groundwater ion concentrations, initial soil and aquifer sediment salt mineral fractions and, due to the study region being a part of the larger Lower Arkansas River Valley, ion mass loading in the Arkansas River at the upstream end of the modeled region (Catlin Dam; see Figure 3B).

307 Salt ion mass loading (kg/day) in the Arkansas River at Catlin Dam were estimated using daily measured values of EC 308 (dS/m) and streamflow (m^3/s) and periodic measurements of salt ion concentration (mg/L). Linear relationships were established 309 between EC and the concentration of each salt ion, with this relationship then used to estimate salt ion concentration for each day 310 of the simulation period. The daily in-stream mass of each salt ion was then calculated by multiplying daily salt ion 311 concentration by streamflow, and added to the point-source SWAT input file for the appropriate subbasin. Figure 4A shows the 312 daily loading (kg/day) for each salt ion using this method. The make-up of total mass loading by salt ion is shown in Figure 4B, 313 with SO_4 accounting for 47% of total in-stream salt mass. The linear relationship between EC and selected salt ions (SO_4 , Cl, Na) 314 and TDS is shown in the charts along the bottom of Figure 4. For TDS the R^2 value of the relationship is approximately 0.93.

315 Initial salt ion concentrations in soil water and groundwater were based on averages of observed groundwater 316 concentrations. For the baseline simulation, the same values were assigned to each HRU. These are 1875 mg/L, 330 mg/L, 175 mg/L, 440 mg/L, 10 mg/L, 150 mg/L, 5 mg/L, and 350 mg/L for C_{SO_4} , C_{Ca} , C_{Mg} , C_{Na} , C_K , C_{Cl} , C_{CO_3} , and C_{HCO_3} , 317 318 respectively. The effect of using spatially-varying initial concentrations is explored in additional scenarios. Salt mineral fractions 319 for CaSO₄ and CaCO₃ in the HRU soil layers are based on a soil survey of the region from the Natural Resources Conservation 320 Service (NRCS). The fraction of soil that is $CaSO_4$ and $CaCO_3$ was set to 0.1 and 0.01, with all others set to 0.0. For the aquifer 321 sediment, fractions are based on the spatial patterns determined in Tavakoli-Kivi et al. (2019) for a salinity groundwater transport 322 study of the same region. Solubility products for precipitation-dissolution of salt minerals were obtained from literature and from 323 Tavakoli-Kivi et al. (2019) and are 3.07 x 10⁻⁹, 4.8 x 10⁻⁶, 4.9 x 10⁻⁵, 0.0072, and 37.3 for CaCO₃, MgCO₃, CaSO₄, MgSO₄, and 324 NaCl, respectively, for both soil and aquifer sediments.

325 Manual calibration was applied to the model to yield correct magnitudes of salt ion concentration in soil water, groundwater, 326 and stream water. Due to the predominance of SO_4 and Ca among salt ions in the regional system, targeted parameters were the 327 solubility product of $CaSO_4$ precipitation-dissolution and the soil fraction of $CaSO_4$. The solubility product was increased from 328 0.000049 to 0.0003, and the soil fraction of CaSO₄ was decreased from 0.01 to 0.009. Model results are tested against in-stream 329 concentration of salt ions, soil salinity, groundwater concentration of salt ions, and groundwater salt ion mass loading to the 330 Arkansas River. For soil salinity, model results are compared with the 54700 ECe values from the field survey. ECe of the soil 331 water in the SWAT model layers for each day of the simulation is estimated using the following steps: 1) soil water TDS is 332 computed by summing up salt ion concentrations in the soil water; 2) soil water EC (EC_w) is computed by dividing soil water 333 TDS by a TDS \rightarrow EC_w (dS/m) conversion of 1020 (mg/L per dS/m) based on soil water samples; and 3) EC_e is computed by 334 multiplying EC_w by the ratio of stored water (mm) to water at saturation (mm) for the SWAT soil layer. Simulated EC_e values 335 are included in the comparison with field-measured EC_e values if the simulated water content of the HRU soil layer is greater

- 336 than 0.07, since Morway and Gates (2012) measured field EC_e only if the soil water content was above this value due to EM-38
- 337 sensors being unreliable at low water contents (Rhoades et al., 1999).
- 338 Several variations of the model were run to test the effect of 1) initial salt ion concentrations in the HRU soil layers and 2) 339 specified loading of salt ion mass at the upstream end of the Arkansas River. For 1), the variations include uniform initial 340 concentrations (baseline model), random spatially-variable concentrations, and initial concentrations equal to 0. For 2), the 341 variation included one simulation with no loading.

342 3.3.2 Model Results

343 3.3.2.1 In-Stream Salt Ion Concentration

Simulated and observed in-stream salt ion concentrations (mg/L) are shown in Figure 5 for the Rocky Ford, Timpas Creek, Crooked Arroyo, and Las Animas sites for each of the 8 ions. Overall, the model tracks the measured concentrations well, particularly for SO₄, Ca, and HCO₃. Results for TDS at all 5 gaging stations are shown in Figure 6, including the Nash-Sutcliffe model efficiency coefficient (NSE) for each site. NSE values are good for Rocky Ford and Crooked Arroyo (0.68 and 0.65), and poor for the other three (< 0.3). However, comparing simulated and measured in-stream concentrations on a daily basis is generally a difficult challenge for watershed modeling.

350 In the two tributaries (Timpas Creek and Crooked Arroyo) and the watershed outlet (Las Animas), the model tends to under-351 predict the ions of low concentration: Mg, K, Cl, and CO₃. The cause for the under-prediction of these ions may be due to the 352 unobserved presence of MgSO4, MgCO3, and NaCl in the soil. These minerals are not observed in NRCS soil surveys of the 353 region, and hence were not included in the baseline model. However, several model scenarios were run to investigate the 354 influence of these minerals. Soil bulk fractions between 0.0001 and 0.0005 were applied for these three minerals, with a large 355 resulting effect on in-stream concentrations of Mg, Na, Cl, and CO₃. For example, using a fraction of 0.0002 resulted in correct 356 magnitude of these four ions at the Las Animas site, but over-estimated concentrations in the tributaries (e.g. Timpas Creek) 357 (Figure 7). This model scenario, however, applied uniform salt mineral fractions of MgSO₄, MgCO₃, and NaCl across all 5270 358 HRUs. Applying spatially-varying fractions across the watershed could provide the correct magnitude of in-stream 359 concentrations of all ions at all stream sampling sites. Regardless, measured in-stream concentrations can provide key 360 information as to the salt minerals present in the watershed, and differences between model output and field data highlight the 361 need for better field survey data of salt mineral content in soils.

362 The in-stream concentrations in the two tributaries (Figure 5B,C) are much more variable than the two sites in the main stem 363 of the Arkansas River. The two tributaries act as drainage channels for irrigation runoff and groundwater return flows, with much 364 lower flows than the Arkansas River, and hence the in-stream concentrations are effected much more strongly by salt loadings 365 from irrigation events and associated flow patterns. In regards to the NSE, the model under-performs for the tributaries (Timpas 366 Creek, Crooked Arroyo), with NSE equal to -0.29 and 0.65, respectively, for TDS (Figure 6B, 6C). However, the overall trends 367 and magnitude compare well to observed data. This is shown in the 1:1 plot of all salt ion data for Timpas Creek in Figure 8B. 368 resulting in an \mathbb{R}^2 value of 0.69. The relationship for Crooked Arroyo yields an \mathbb{R}^2 value of 0.80 (not shown). This is particularly 369 promising given that there is no specified upstream loading for the tributaries, and hence all salt mass within the stream system is 370 due to surface runoff, lateral flow, and groundwater discharge. Hence, comparing simulated and observed in-stream salinity 371 concentration in these two systems provides a strong test for the model.

The summary of in-river salt concentration results is shown by a 1:1 comparison of all salt ion data for the Rocky Ford (Figure 8A) and Las Animas (Figure 8C) sites, which yield R^2 values of 0.87 and 0.66, respectively. Timpas Creek (Figure 8B) has an R^2 value of 0.69. However, as the SWAT model often is used to estimate monthly in-stream loads rather than daily instream concentration, these results are promising regarding the use of SWAT to estimate in-stream salinity loadings. 376 Figure 9 shows the salt loading via the hydrologic pathways of groundwater discharge (Figure 9A), surface runoff (9B), and 377 percolation from the soil profile to groundwater (9C). For Timpas Creek, 96% of salt in the creek water is from groundwater 378 discharge, 3% from surface runoff, and 1% from lateral flow. For Crooked Arroyo, the portions are 91%, 6%, and 3%, and for 379 the Arkansas River they are 96%, 3%, and 1%, highlighting the strong influence of groundwater on surface water salt load. This 380 is shown further by examining the domain-wide salt balance, presented in Sect. 3.3.2.3. The mass loading of total salt from the 381 aquifer to the Arkansas River for each day of the 2006-2009 time period is shown in Figure 10. Mass balance plot values are the 382 mean of a stochastic river mass balance calculation of surface water salinity loadings along the length of the Arkansas River 383 within the model domain, using a method similar to Mueller-Price and Gates (2008), with values indicating the mass of salt not 384 accounted for by surface water loadings. These unaccounted for loadings include groundwater, and thus provide an upper limit of 385 in-stream salt loading from groundwater discharge.

386 3.3.2.2 Groundwater and Soil Water Salinity

387 Groundwater salt results are shown by spatial maps and by comparison of frequency distributions. For all simulated results, 388 only concentration values from days on which field samples were taken are included in the analysis. Time-averaged TDS (mg/L), 389 SO₄ (mg/L), and Na (mg/L) in groundwater is shown for each HRU in Figure 11. Also shown is soil water EC (dS/m) for each 390 HRU soil profile, and the percent of the soil profile (Figure 11E) and aquifer (Figure 11F) that is CaSO₄ (solid mineral) at the 391 end of the simulation period. These maps are shown to provide an indication of the degree of spatial variation simulated by the 392 model. Variation in each system response is large, with TDS ranging from 0 to ~11,700 mg/L, SO₄ from 0 to ~6700 mg/L, and 393 Na from 0 to ~1270 mg/L. In comparison, if data from an outlier monitoring well are excluded (monitoring well with salinity 394 values more than double of any other monitoring well), the maximum observed values for TDS, SO₄, and Na are 13000 mg/L, 395 6500 mg/L, and 2600 mg/L.

Results for all salt ions are summarized in Table 2. Average concentration of field samples (based on field samples from 82 monitoring wells shown in Figure 3B) and HRU-simulated groundwater salinity compares well, particularly for SO₄ (1878 mg/L to 2149 mg/L) and for TDS (3334 mg/L to 3508 mg/L). In addition to a comparison of maximum and average values, comparison at various magnitude levels is performed using relative frequency plots, shown in Figure 12. Results for SO₄ (Figure 12A), HCO₃ (12B), and TDS (12C) are shown. Similar to the results shown in Table 2, the comparison for SO₄ and TDS is good, but the model generally under-predicts HCO₃ for most HRUs.

402 A relative frequency plot of observed and simulated EC_e (dS/m) in the soil profile is shown in Figure 12D. The simulated 403 values were taken from HRUs coinciding with cultivated fields for the days of April 15, May 15, June 15, July 15, and August 404 15, for the years 2001-2005. Note that simulated values were taken from each cultivated HRU, whereas the field surveys using 405 the EM-38 sensors were conducted in approximately 100 fields. The average of observed values is 4.1 dS/m, although this 406 number is skewed by extremely high values (> 30 dS/m). If only values < 6.5 dS/m are considered (89% of the samples), then the 407 average is 3.2 dS/m. The average of the simulated values is 2.96 dS/m. As seen from the frequency distribution in Figure 12D, 408 the model tends to under-estimate soil salinity for some of the HRUs, and does not capture the high salinity values (> 7 dS/m). 409 However, the overall magnitude and distribution of values approaches the distribution of the measured values. Note that EM-38 410 measurements have inherent uncertainty. In addition, some of the HRUs included in the analysis are fallow during this period 411 (2002-2005), which may lead to low soil salinity values that were not measured in the field survey.

412 **3.3.2.3** Salt Balance

The domain-wide salt balance is presented in Figure 13A. All salt balance components are included, with all values scaled according to the small salt flux (lateral flow = 1 unit). For the soil profile, salt is added via groundwater irrigation (17 units), surface water irrigation (29), dissolution of salt minerals (97), and upflux from the aquifer saturated zone (44), and removed via 416 percolation (134), surface runoff (3), and lateral flow (1). A similar salt balance can be performed for each salt ion in the system.

417 Salt removed from the aquifer and added to the soil profile via upflux is approximately 30% of percolation, which compares well 418 to a comparison of water upflux and recharge magnitudes computed by Morway et al. (2013) in a groundwater modeling study of

419 the region using MODFLOW.

420 Of the salt entering the river, 97.6% is from groundwater (162 units out of 166), and the remaining from surface runoff and 421 lateral flow. Time series of daily loading (kg/ha) for these three components is shown in Figure 13B, and loadings for 422 percolation, surface water irrigation, and groundwater irrigation are shown in Figure 13C, showing the seasonal trends in 423 applying irrigation water. Notice that the highest groundwater loading rates coincide with the "spikes" in the in-stream 424 concentration plots of Figures 5 and 6, indicating the strong influence of groundwater loading on in-stream salt concentrations. 425 The fluctuations in simulated in-stream concentration, however, are larger than observed with the measured values. This is due to 426 the manner in which SWAT simulates groundwater return flow, with a steady-state flow equation for each HRU that provides 427 pulses of groundwater to streams rather than the multi-dimensional groundwater flow equation that provides physically-based, 428 spatially-distributed diffuse flow through the aquifer towards the stream network.

Results in Figure 13C indicate that much of the salt leaching from the soil profile is due to dissolution of salt minerals. Results also indicate the importance of including salt mass in applied irrigation water, as it accounts for approximately half of salt leaching to the aquifer. Finally, results show the importance of including precipitation-dissolution in the module, as this process is a large component of the salt balance. Without including this process, the module would severely under-predict salt ion concentrations throughout the watershed, demonstrating the need to include each salt ion individually as opposed to modeling salinity as a conservative solute in the system.

435 3.3.2.4 Scenarios and Model Guidelines

The effect of initial salt ion concentrations and upstream salt ion mass loading is summarized by the time series charts in Figure 14. For the Rocky Ford and Las Animas gaging sites, a time series of simulated TDS (mg/L) is compared for the following scenarios: uniform initial salt ion concentration ("Original": this refers to the baseline simulation); HRU-variable initial concentration ("Variable IC"); initial concentrations equal to 0 ("Zero IC"); and not accounting for upstream salt ion mass loading at Catlin Dam ("No US Loading"). There are only small differences between using uniform or HRU-variable initial concentrations for soil water and groundwater. Any differences are readily resolved during the warm-up period. Hence, to facilitate model use we recommend that uniform initial concentrations be used.

443 Using initial concentrations equal to 0 mg/L has a significant effect, particularly for downstream sites such as Las Animas 444 (Figure 14C,D). For this watershed, salt loading to the streams is principally from groundwater, and if soil water and 445 groundwater are not provided with initial salt ion concentrations, the groundwater salt ion loading to subbasin streams is small 446 compared to the baseline simulation. As downstream flow and in-stream salt loading is effected by groundwater loading, these 447 areas (e.g. Las Animas site) experience the effect more acutely than upstream sites such as Rocky Ford (Figure 14A,B). 448 However, by the end of the simulation (2009), difference between "Zero IC" and "Original" is small. This is shown by the "Diff" 449 time series for each plot. Therefore, if groundwater discharge is a large component of total water yield for the watershed, "Zero 450 IC" should not be used, or a long warm-up simulation period needs to be used.

Not including upstream salt ion loading at Catlin Dam has a stronger effect on the Rocky Ford site (Figure 14A,B) than at the outlet (Las Animas) (Figure 14C,D). This is due to Las Animas being much farther downstream, and hence there is much more groundwater salt ion loading to the streams that can make up for the salt not included at the upstream end of the Arkansas River at Catlin Dam. Overall, any point sources of in-stream salt should be added, unless only downstream areas are targeted for

- 455 baseline simulations and best management practice investigation. The effect of neglecting point sources of in-stream salt 456 decreases as the groundwater loading component of total salt yield increases.
- 457 The importance of including equilibrium chemistry into the salt transport module is demonstrated by the results shown in 458 Figure 15. The simulated in-stream TDS (mg/L) is shown at the Rocky Ford site (Figure 15A), the Timpas Creek site (B), and 459 the Las Animas site (C), for both the original simulation (red line) and a simulation "No SEC" that does not include the SEC 460 module (black line). The "No SEC" simulation therefore represents a system wherein salt is transported through the stream-461 aquifer system as a conservative species. Clearly, in-stream concentrations are much too low for the simulation without the SEC 462 module for the Timpas Creek and Las Animas sites. This is due to the neglect of salt mineral dissolution, which in the actual 463 system transfers salt mass from the soil and aquifer material to soil water and groundwater are thereby increases the loading of 464 salt to the stream network. For the Rocky Ford site, the scenarios yield similar results due to the location of the site being close to 465 the upstream end of the modeled region, and thus in-stream concentrations are not affected by groundwater and surface runoff 466 salt loadings to the river. For this system, and likely most watersheds, equilibrium chemistry must be included to establish the 467 correct magnitude of salt loading and concentrations.

468 **3.3.3 Model Use and Limitations**

469 The salinity module of SWAT differs from other salinity models in that it accounts for salt loading for each major 470 hydrologic pathway in a watershed setting (stream, groundwater, lateral flow, surface runoff, tile drain flow), for each major salt 471 ion, subject to chemical equilibrium reactions (precipitation-dissolution, complexation, cation exchange). As such, it can be used 472 to estimate baseline salt loading within a watershed, and also explore the impact of land management and water management 473 scenarios to mitigate soil salinity, groundwater salinity, and surface water salinity. The model, however, does not simulate 474 physically-based, spatially-distributed groundwater flow and solute transport with an accurate depiction of water table elevation 475 and groundwater head gradient, and thus the trends in groundwater salt loading to streams may not be accurate (see Figure 9). To 476 overcome this issue, the new salinity module could be incorporated into SWAT-MODFLOW (Bailey et al., 2016), which links 477 SWAT and MODFLOW to simulate land surface and subsurface flow processes, and SWAT-MODFLOW-RT3D (Wei et al., 478 2018), which includes reactive transport of solutes into SWAT-MODFLOW.

479

480 4 Conclusions

481 This study presents a new watershed-scale salt ion fate and transport model, by developing a salinity module for the SWAT 482 model. The module accounts for salt loading for each major hydrologic pathway in a watershed setting (stream, groundwater, 483 lateral flow, surface runoff, tile drain flow), for each major salt ion (SO₄, Ca, Mg, Na, K, Cl, CO₃, HCO₃). The module also 484 accounts for principal equilibrium chemistry reactions (precipitation-dissolution, complexation, cation exchange). For 485 precipitation-dissolution, five salt minerals (CaSO₄, CaCO₃, MgCO₃, NaCl, MgSO₄) have been included. The model was applied 486 and tested in a 732 km² irrigated stream-aquifer watershed in southeastern Colorado, along the alluvial corridor of the Arkansas 487 River. Model results are tested against in-stream salt ion concentration, groundwater salt ion concentration, soil salinity, and 488 groundwater salt loading to the Arkansas River.

The model can be used to assess baseline salinity conditions in a watershed and to explore land and water management strategies aimed at decreasing salinization in river basins. Such strategies may include on-farm management, lining irrigation canals to reduce saline canal seepage, dry-drainage practices, and reducing volumes of applied irrigation water. Due to the simulation of soil water salt ion concentrations and SWAT's simulation of crop growth, the salinity module can also be used to investigate the effect of these strategies on crop yield. Although this study applied the model to an irrigated area, the model can be applied to non-irrigated areas as well.

496

497 Code Availability

498 The code consists of the original SWAT files, with 6 additional files for the salinity module. All files are *.f FORTRAN files.
499 The code is available on GitHub (<u>https://github.com/rtbailey8/SWAT_Salinity/</u>). The code can also be sent via request from
500 Ryan Bailey at rtbailey@colostate.edu.

501

502 Author Contribution

503 Ryan Bailey wrote the salinity module for SWAT and tested the module for the study region. Saman Tavakoli-Kivi prepared the 504 solution chemistry algorithms for the salinity module. Xiaolu Wei prepared and tested the original SWAT model for the study 505 region, and facilitated use of the new salinity module for the constructed SWAT model.

506

507 **Competing Interests**

508 The authors declare that they have no conflict of interest.

509

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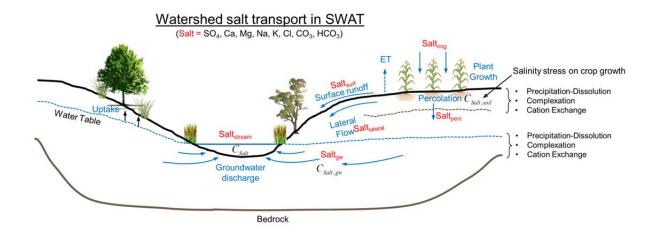


Figure 1. Schematic showing a cross-section of an irrigated stream-aquifer system and the major transport pathways of salt,

which consists of the eight major ions of SO₄, Ca, Mg, Na, K, Cl, CO₃, HCO₃. The concentration of each ion is also governed by

equilibrium chemistry reactions such as precipitation-dissolution, complexation, and cation exchange within the soil profile and

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within the aquifer.

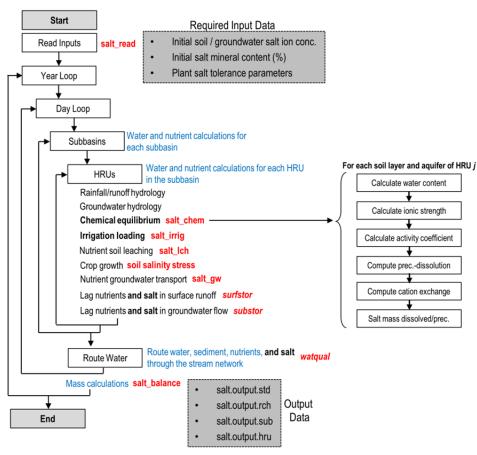


Figure 2. Data flow within the SWAT-Salt modeling code. Boxes and text in black and blue indicate original SWAT loops and subroutines. Text in red indicates either new or modified subroutines for the Salinity module. The required input data for the salinity module is shown in the upper shaded box, whereas the generated output files are shown in the lower shaded box.

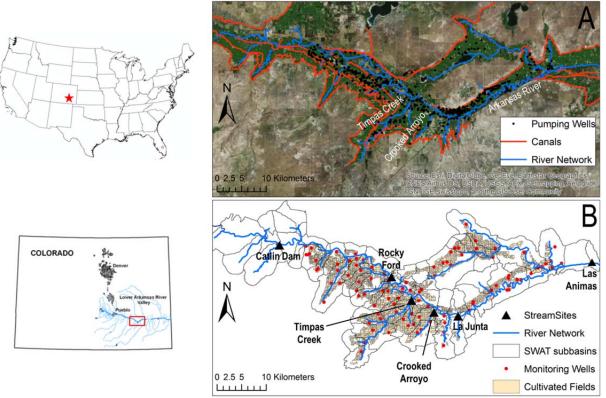


Figure 3. Map of study region within the Lower Arkansas River Valley of Colorado, showing (A) Arkansas River and tributaries, irrigation canals, and pumping wells, and (B) cultivated fields, monitoring wells where groundwater is sampled for salt ions, sampling sites where surface water is sampled for salt ions, and SWAT subbasins.

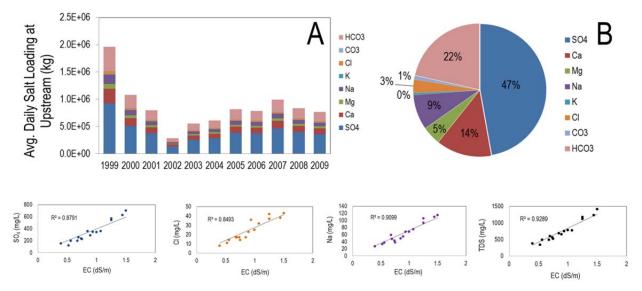


Figure 4. Data summarizing the specified loading of salt (kg/day) at the Catlin Dam gage site, using observed EC (dS/m) and stream discharge (m³/day) data: (A) daily loading of salt ion, (B) percentage of total salt loading attributed to each salt ion, (bottom charts) example regression plots used to relate EC to salt ion concentration.

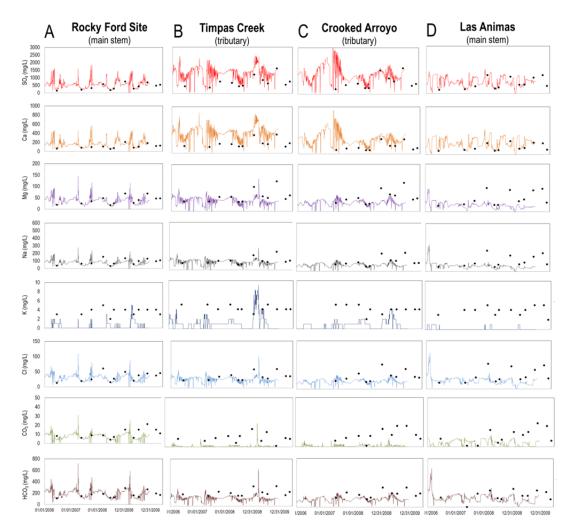


Figure 5. Time series of simulated and observed concentration (mg/L) for each of the 8 major salt ions for the (A) Rocky Ford site, (B) Timpas Creek site, (C) Crooked Arroyo site, and (D) Las Animas site. Simulated hydrographs for these sites are in Wei et al. (2018).

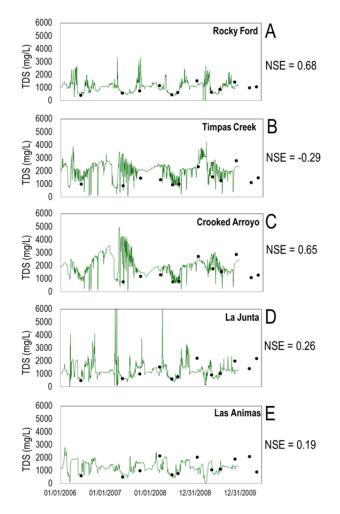


Figure 6. Simulated and observed total dissolved solids (TDS) (mg/L) in the five stream sampling sites along the Arkansas River
(A, D, E), and two tributaries (B, C). See Fig. 3 for locations. TDS is the summation of the concentration of the 8 salt ions. The
Nash-Sutcliffe model efficiency coefficient (NSE) is shown for each plot.

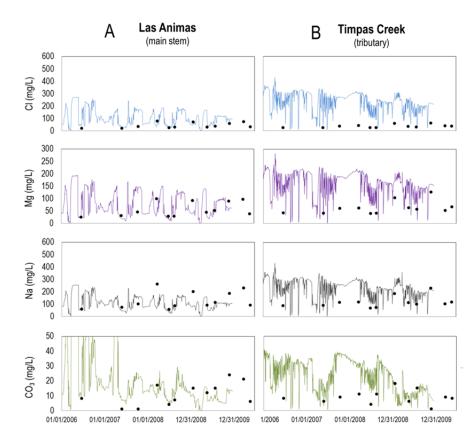


Figure 7. Time series of simulated and observed concentration (mg/L) for each of the 8 major salt ions for the (A) Las Animas site and (B) Timpas Creek site, for the model scenario of using 0.0002 soil bulk fractions for MgCO₃, MgSO₄, and NaCl. For the baseline model, these fractions were set to 0.00.

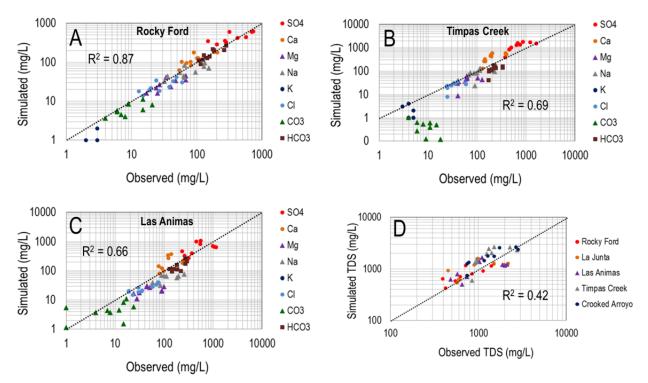
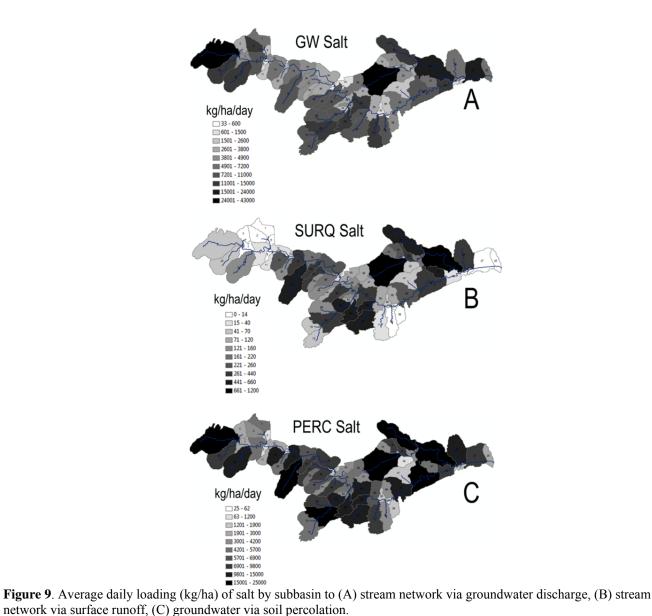


Figure 8. Log-log plots of observed vs. simulated salt ion concentration for the (A) Rocky Ford, (B) Timpas Creek, and (C) Las Animas surface water sampling sites. (D) shows the comparison of TDS for the five sites.



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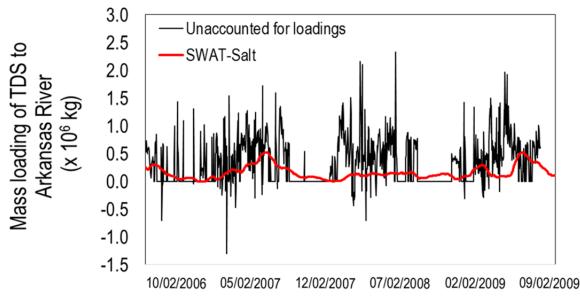


Figure 10. Simulated daily mass loading of TDS (kg) to the Arkansas River via groundwater discharge for the SWAT model with uniform initial salt concentrations. Results from a salt mass balance calculation on the Arkansas River also are plotted, showing the unaccounted for TDS loadings (groundwater, surface runoff, small inflows) in the Arkansas River.

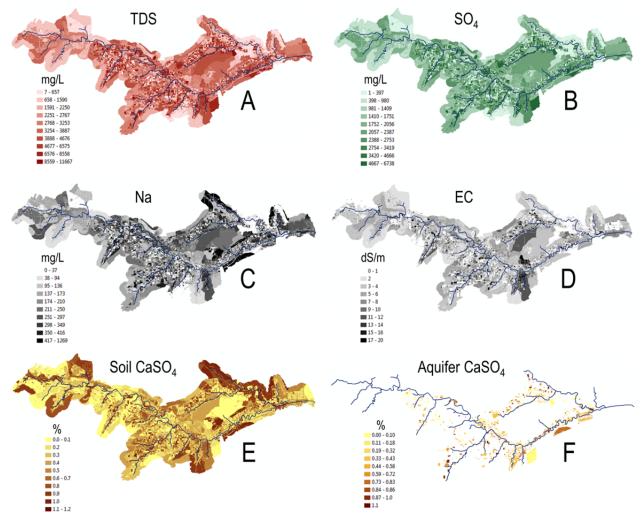


Figure 11. HRU average concentration over the 2006-2009 simulation period for (A) groundwater TDS (mg/L), (B) groundwater SO₄ (mg/L), (C) groundwater Na (mg/L), and (D) soil water electrical conductivity EC (dS/m). (E) and (F) show percentage of soil bulk volume and aquifer bulk volume, respectively, that is CaSO₄, near the end of the simulation in May 2010.

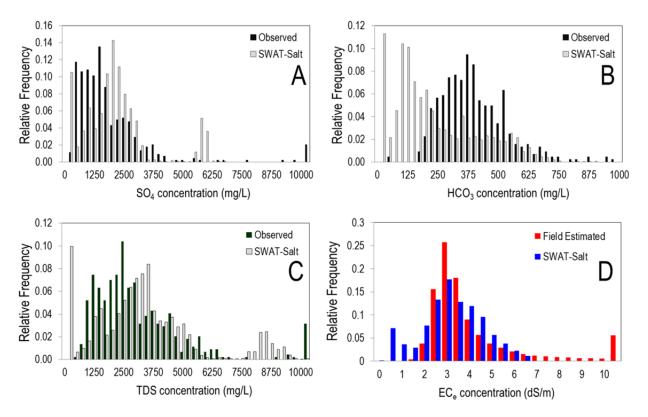


Figure 12. Relative frequency plots of simulated and observed values of (A) SO_4 groundwater concentration, (B) HCO_3 groundwater concentration, (C) TDS groundwater concentration, and (D) EC_e soil water concentration of a saturated paste. Groundwater simulated values are taken from each HRU of the SWAT simulation, on days for which observed values are available. For soil EC_e , values are taken only from HRUs that coincide with cultivated fields.

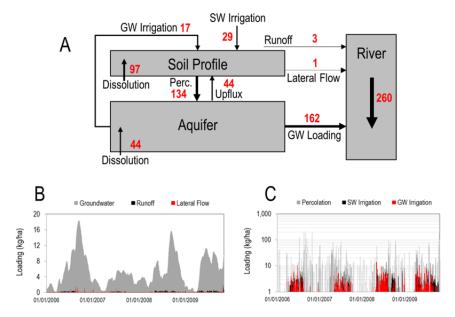
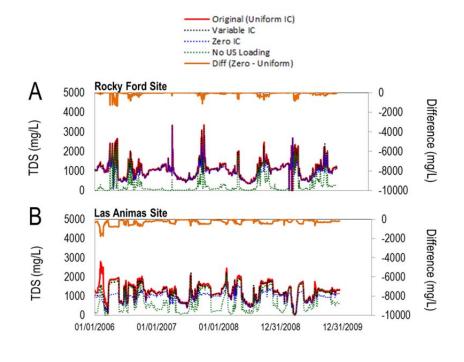


Figure 13. Magnitude of salt balance components in the watershed model for TDS, showing (A) relative salt flux between soil storage compartments in the watershed for each salt transport pathway; (B) daily loading (kg/ha) of salt in groundwater, surface runoff, and lateral flow to streams; and (C) daily loading (kg/ha) of salt in percolation water (from bottom of soil profile to the aquifer), irrigation derived from irrigation canals, and irrigated derived from groundwater pumping.



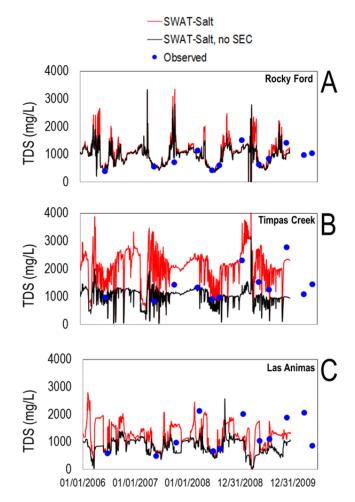
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between the IC = 0 scenario and the original scenario.

Figure 14. Simulated in-stream TDS concentration (mg/L) at the Rocky Ford and Las Animas gage sites along the Arkansas

original simulation; variable IC; IC = 0; and no upstream loading of salt at the Catlin Dam site. Also show is the difference

River for four scenarios: uniform initial conditions (IC) of salt soil water and groundwater concentrations, corresponding to the



843 844 845 846 847 Figure 15. Simulated in-stream TDS concentration (mg/L) at the (A) Rocky Ford Site, (B) Timpas Creek Site, and (C) Las Animas Site for the original simulation (red line) and a simulation without including equilibrium chemistry (SEC module) (black line). The measured TDS values also are shown.

Table 1. Groups and Species included in the Salinity Equilibrium Chemistry (SEC) module for SWAT.

Group	Species
Aqueous Species	Ca ²⁺ , Mg ²⁺ , Na ⁺ , K ⁺ , SO ₄ ⁻² , CO ₃ ²⁻ , HCO ₃ ⁻ , Cl ⁻
Solid Species	CaSO4,CaCO3,MgCO3,NaCl, MgSO4
Complexed Species	$CaSO_4^0$, $MgSO_4^0$, $CaCO_3^0$, $CaHCO_3^+$, $MgCO_3^0$,
complexed species	MgHCO ⁺ ₃ , NaSO ⁻ ₄ , KSO ⁻ ₄ , NaHCO ⁰ ₃ , NaCO ⁰ ₃
Exchanged Species	

Table 2. Summary statistics for observed (monitoring well) and simulated (SWAT) salinity concentrations in groundwater.

Maximu		m (mg/L)	Average (mg/L)	
Species	Observed	Simulated	Observed	Simulated
Na	2606	677	402	247
Ca	767	2233	353	628
Mg	1019	341	191	117
K	85	353	4	6
SO4	6510	6132	1878	2149
CO3	42	4	2	0
HCO3	2362	1232	410	299
Cl	1803	225	95	63
TDS	13007	9920	3334	3508