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# Improving Modeling of Quinoa Growth under Saline Conditions Using the Enhanced Agricultural Policy Environmental eXtender Model

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**Abstract:** Cultivation of highly salt-tolerant plants (i.e., halophytes), may provide a viable alternative to increase productivity compared to conventional salt-sensitive crops, increasing the economic potential of salt-affected lands that comprise ~20% of irrigated lands worldwide. In this study the Agricultural Policy/Environmental eXtender (APEX) model was adapted to simulate growth of the halophyte quinoa, along with salt dynamics in the plant-soil-water system. Model modifications included salt uptake and salt stress functions formulated using greenhouse data. Data from a field site were used to further parameterize and calibrate the model. Initial simulation results were promising, but differences between simulated and observed soil salinity and plant salt values during the growing season in the calibration suggest that additional improvements to salt uptake and soil salinity algorithms are needed. To demonstrate utility of the modified APEX model, six scenarios were run to estimate quinoa biomass production and soil salinity with different irrigation managements and salinities. Simulated annual biomass was sensitive to soil moisture, and root zone salinity increased in all scenarios. Further experiments are needed to improve understanding of crop salt uptake dynamics and stress sensitivities so that future model updates and simulations better represent salt dynamics in plants and soils in agricultural settings.

Keywords: salinity; APEX model; irrigation management; halophyte

## 1. Introduction

Soil salinity is a major problem in (semi)-arid regions where evapotranspiration (ET) exceeds precipitation. Salinity negatively impacts crop productivity in nearly 20% of irrigated agricultural lands worldwide [1]. This percentage is expected to grow with increasing desertification, endangering the ability to provide enough food for growing human populations, especially in areas where food supplies are already scarce. Natural processes contribute to soil salinization, and management activities including irrigation with saline water can exacerbate this problem. Salinity can damage plants through reductions in osmotic potential and accumulation of toxic ions in plant tissue [2]. Tolerance to salinity varies by crop and cultivar, but typical thresholds for common crops are between 1 dS/m for sensitive crops and 7–8 dS/m for more tolerant crops [3]. Soils with salinities greater than 4 dS/m are considered saline [4].



Detrimental effects of soil salinity on crop production can be managed by leaching salts below the root zone, sometimes in combination with amendments such as gypsum if salts are dominated by sodium (Na<sup>+</sup>). However, these management options may be limited in regions where access to freshwater or amendments is inadequate. Cultivation of salt-tolerant crops may provide a means to use salt-affected lands. Highly salt-tolerant plants, known as halophytes, have been successfully cultivated on saline soils with yields equivalent to those of conventional crops grown in non-saline soils [5,6]. Halophytes comprise 1% of plant species [7] and can thrive in saline environments by utilizing a range of strategies including salt exclusion at the root-soil interface, salt sequestration within plant tissues, and salt excretion. Several halophytic crops have shown promise for human consumption, animal feed and forage, biofuels and fuelwood [5,8]. An added benefit of cultivating halophytes could be that, when harvested, salt contained in the crop is removed from the system, potentially providing a means to remediate salt-affected soils.

One halophyte that has recently received attention is quinoa (*Chenopodium quinoa* Willd.). Traditionally cultivated from sea level to nearly 4000 m in elevation, quinoa has a large genetic diversity [9,10]. Quinoa seeds and greens can be consumed by humans, while harvest residues can be consumed by animals [11]. Along with its high nutritional value, quinoa's drought and salt tolerance have contributed to its increased popularity as a commercial crop [9,12]. Under optimal management, 3–5 t/ha of grain can be produced [13]. Although some varieties can survive salinities greater than 40 dS/m, responses to saline conditions vary by cultivar, with optimal salinities ranging from 10 to 20 dS/m [10,12].

Simulation modeling can be used to explore quinoa growth in specific locations and climates, and to determine potential long-term impacts of quinoa cultivation on soil and water. To date, however, few studies have modeled halophytic crops. Kaya et al. [14] simulated dry matter and grain yield of quinoa (var. Titicaca) growth under saline irrigation treatments in a Mediterranean setting using the SALTMED model. Vermue et al. [15] used SWAP to simulate production and transpiration of sea kale (*Crambe maritima* L.) and long-spiked glasswort (*Salicornia dolichostachya* Moss) under drought and salinity stress in the Netherlands. Ben Asher et al. [16] also used SWAP to examine the effects of using halophytes in rotation with salt-sensitive crops under saline irrigation. In addition to examining crop yield and transpiration as in Kaya et al. [14] and Vermue et al. [15], Ben Asher et al. [16] simulated salt uptake and soil salt distribution.

Simulation models that integrate salinity dynamics vary greatly in complexity, scale, and approach. Several models, including MOPECO-Salt [17], SALTMED [18], SWAP [19,20], and ENVIRO-GRO [21], contain a salt stress component, but differ in how salt stress is applied. In most models, empirical relationships between salinity and water potential are used to calculate reductions in water uptake with increased salinity [22].

In this paper, we describe modifications made to the Agricultural Policy/Environmental eXtender (APEX) model to include simulation of processes related to salt in plants and soils using experimental data from greenhouse and field studies. APEX simulates crop growth and water and nutrient transport at a watershed scale [23]. The model accounts for salt movement in the soil, but currently does not simulate salt-induced osmotic stress and plant salt uptake. The main objectives of this paper are to (1) describe modifications to APEX to include crop-specific salt uptake and salt stress; (2) describe calibration of the enhanced APEX model with data from ongoing field studies with quinoa; and (3) demonstrate utility of the updated model for long-term simulations of quinoa crop management.

### 2. Materials and Methods

#### 2.1. Model Description

APEX is a physically-based farm- to small watershed-scale model. APEX explicitly simulates management practices such as tillage and fertilization, taking into account water, soil, erosion, and pest characteristics [23]. Using a daily time step, APEX can complete simulations spanning centuries.

Crop growth directly depends on radiation and can be limited by water and nutrient deficiencies, temperature, and salt stress [23]. A detailed description of major model components is provided by Gassman et al. [24] and Williams et al. [23]. Parameters and variables pertinent to our study are listed in Supplemental Table S1. Prior to our modifications, the model simulated total salt content of fertilizer, irrigation water, soil water, runoff, and leaching [25], and no distinction is made between different ions.

#### 2.1.1. Plant Salt Uptake

We created the SLTUSE subroutine to calculate plant salt uptake. Data from mature greenhouse-grown quinoa were used to establish an empirical relationship between soil salinity and plant uptake. A mechanistic approach was not used because mechanisms for salt uptake and allocation in quinoa are still poorly understood [2,6]. Tissue salt concentration was calculated as the sum of Na<sup>+</sup>, potassium (K<sup>+</sup>), calcium (Ca<sup>2+</sup>), magnesium (Mg<sup>2+</sup>), sulfate (SO<sub>4</sub><sup>2-</sup>), and chlorine (Cl<sup>-</sup>) concentrations.

The greenhouse study (Appendix A) showed that leaf salt concentrations increased linearly with soil salinity (Figure 1; Equation (1),  $R^2 = 0.97$ , n = 5). Because irrigation treatments added salt to the pots over time, initial and calculated final (initial plus salts added via irrigation) soil salinities were averaged for each salinity treatment. Average plant salt concentrations at each average soil salinity were used for the regression analysis. Average soil salinities in the greenhouse study ranged from 2.4 to 12.4 dS/m, and we extrapolated the regression for salinities greater than 12.4 dS/m. Because no salt can be taken up by plants when no salt is available in the soil, a separate linear equation was used for salinity levels between 0.0 and 2.0 dS/m (Equation (2)).

Plant Salt Concentration (ppm) = 
$$(2612.7 \times \text{average soil salinity}) + 86370$$
 (1)

for soil salinity  $\geq 2.0 \text{ dS/m}$ 

Plant Salt Concentration (ppm) = 
$$(45797.7 \times \text{average soil salinity})$$
 (2)

for 0 dS/m < soil salinity < 2.0 dS/m.

Plant salt concentrations adjust daily using Equations (1) and (2) to account for daily changes in soil salinity. If the target plant salt content on a given day estimated by Equations (1) and (2) is lower than the actual plant salt content on the previous day due to a reduction in soil salinity, the model assumes that no salt will be taken up until either biomass increases to a point where more salt is needed to reach the target concentration, or soil salinity increases to make the target plant salt content greater than the actual plant salt content. If actual water uptake is less than the model's calculated potential uptake amount, then salt uptake is scaled back proportionally to actual water uptake.

Daily salt uptake is partitioned between different soil layers. The fraction of uptake from each layer is equal to the product of water uptake (mm) and salt (kg/ha) in a soil layer divided by the sum of the products for all root zone soil layers. A maximum daily uptake limit is imposed to control the amount of salt taken up by a plant in the case of a large increase in solution salinity. The maximum value is equal to the lesser of the product of solution salinity by the amount of water uptake (i.e., salt uptake without ion exclusion) or the amount of salt uptake that provides the tissue target concentration.



**Figure 1.** Measured and modeled salt uptake and salt stress for quinoa based on greenhouse study. Straight lines represent the salt uptake algorithms (Equations (1) and (2)), based on average salt concentration in monitored greenhouse plant dry matter in each soil salinity treatment. The pre-calibration salt stress curve (Equation (3)) is fit to the relative biomass of monitored greenhouse plants with STX1 (wavelength parameter) = 12.8 and STX2 (optimal soil salinity for crop growth) = 10.5. Salt stress ranges from 0 to 1, where 1 equals the greatest biomass (no stress).

## 2.1.2. Salt Stress

We added a halophyte-specific salt stress function to APEX based on the response of quinoa to soil salinities tested in the greenhouse experiment. For glycophytes, the model uses a piecewise linear function to calculate salt stress (i.e., [3]). To better represent the growth response of halophytes to soil salinity, we used an empirically-derived sine curve. The stress level ranges continuously from 0 to 1, with 0 indicating full stress and 1 indicating no stress. Three parameters determine the salt stress value: actual soil salinity, optimal soil salinity, and a shape factor (Equation (3)).

Stress factor = 
$$sin[((EC/STX1) \times (1.5708)) - ((1.5708) \times (STX2 - STX1)/STX1)]$$
 (3)

where EC is soil salinity (dS/m), STX1 is the shape factor, and STX2 is the optimal soil salinity (dS/m) at which no plant stress occurs due to salt. The constant 1.5708 is the number of radians in 90 degrees. At optimal soil salinity, the stress factor equals 1.0 (Figure 1). At soil salinities above or below the optimal value, the fraction of growth declines at a rate defined by the shape factor. Daily potential growth is reduced by a factor of (1—stress factor). In this study, STX1 and STX2 were determined by manually adjusting the values in Equation (3) until a good fit was achieved based on the greenhouse experiment data for quinoa. It is important to note that these factors may vary by plant species.

APEX tracks salt in soils in kg/ha but Equations (1) to (3) use units of dS/m. Equation (4) converts salt from kg/ha to dS/m based on the measured relationship between EC and salt amounts in soil layers using the saturated paste extract method [26].

$$CSLT = (0.07 \times WSLT)/(BD \times h)$$
(4)

where CSLT is salinity (dS/m), WLST is soil salt (kg/ha), BD is soil bulk density (g/cm<sup>3</sup>), and h is soil depth (mm).

#### 2.2. APEX Model Setup

#### 2.2.1. Quinoa Parameterization

To parameterize APEX for quinoa, crop characteristics were collected from literature, field and greenhouse data. We used data from the field plot at Main Station Field Lab (MSFL; Appendix B) in 2016 and the greenhouse study to parameterize quinoa under stress-free conditions. Parameters derived from field samples include those mainly related to leaf development and plant density effects on growth (RLAD, DMLA, DLAI, DLAP1, DLAP2, and HMX, PPLP1, and PPLP2; Supplemental Table S1). Salt stress curve shape factor (STX1) and optimal soil salinity (STX2) were initially set based on greenhouse experiment results (Figure 1). Several crop parameters (i.e., TOP, TBS, RBMD, and RLAD; Supplemental Table S1) were adjusted during model runs to improve agreement between simulated and observed biomass on harvest day and the maximum LAI for 2016. Potential heat units (PHU; degree days [DD] needed for a crop to reach maturity [25] was set to 1472 DD based on average daily 2016 growing season temperatures (TBS) and the model's calculated crop fraction of maturity at harvest. Plant population density (OPV5) was set to 61 plants/m<sup>2</sup> based on the average plant density in the field plot. Other initial parameter values were based on personal communication with J. Kiniry [27].

#### 2.2.2. Soil Parameterization

Soil parameters for the MSFL field site were estimated using field measurements and the NRCS Soil Survey Geographic Database (SSURGO). Soils at MFSL belonged to the Truckee series (fine-loamy, mixed, superactive, mesic Fluvaquentic Haploxerolls). The soil was divided into six layers: Layer 1 (0.00–0.01 m), Layer 2 (0.01–0.19 m), Layer 3 (0.19–0.31 m), Layer 4 (0.31–0.49 m), Layer 5 (0.49–1.00 m), and Layer 6 (1.00–1.52 m). Depths of the second and fourth layers were set so that soil salinity and moisture sensors installed at the field site were located in the center of each layer.

#### 2.2.3. Weather Inputs

We used daily solar radiation, maximum and minimum temperature, precipitation, relative humidity, and wind speed data for 2016 collected at MSFL. Some APEX calculations use monthly weather statistics. Because MSFL did not begin weather data collection until 2010, long-term monthly weather data were used from the Reno-Tahoe International Airport (RTIA) approximately 3 km from the MFSL.

#### 2.2.4. Management Inputs

Management activities for calibration and scenario analyses are shown in Figure A1. Irrigation volumes and frequency matched irrigation practices conducted in the 2016 field study. Tillage operations specified in the operations file included tillage, seeding, irrigation, and harvesting. No fertilizer was applied during the 2016 season.

#### 2.3. Model Calibration

APEX was calibrated to field plot conditions and quinoa growth using parameters determined to be sensitive in a sensitivity analysis (see Appendix C and Supplemental Table S1). We used seven quinoa sampling events to compare simulated with measured STL, LAI, and USLT. Soil sensors provided hourly measured SW2 and WSLT2 data starting July 8. Calibration occurred in two stages: first we focused on crop growth and soil water parameters, then we continued with salt-related parameters. For calibration, we randomly assigned values within a designated range for each calibration parameter. Parameters that showed no sensitivity and parameters for which we had reliable data were not included in calibration.

In the first calibration stage, crop biomass-energy ratio (WA) and soil saturated hydraulic conductivity (SATC) were adjusted. For each run, observed field values of STL, LAI, and SW2 were compared to simulation results. Using WA and SATC values that produced the best set of metrics from the 200 runs completed in the first stage, the second calibration stage involved performing an additional 200 runs that adjusted STX1, STX2, Parm86, and ECND. In addition to calculating statistics for STL, LAI, and SW2, statistics were calculated for USLT and WSLT2 in the second calibration stage. The best-fit parameter set was chosen based on the best set of calibration metrics.

#### 2.4. Long-Term Scenarios

We created six long-term scenarios to assess the potential long-term impacts of irrigation quantity and different soil salinities on quinoa production and the salt balance in the plant-soil system (Table 1). In addition to simulating irrigation levels for 2016 (MID), irrigation volumes were adjusted to either double (HI) or half (LO) of 2016 levels across 15-year periods. Irrigation water salinity was increased from 420 ppm (value used in 2016 simulations based on irrigation water available for the field experiment; NS) to 3000 ppm (S). The latter value was derived from irrigation water salinity measured in Uzbekistan [28] and other locations [29].

**Table 1.** 15-year scenarios based on three irrigation levels: low, mid, and high (LO, MID, and HI) and two irrigation salinities, non-saline (NS) and saline (S). The MID-NS scenario represents conditions in the field experiment.

Scenario Code	Annual Irrigation (mm)	Irrigation Salinity (ppm)
LO-NS	272	420
MID-NS	544	420
HI-NS	970	420
LO-S	272	3000
MID-S	544	3000
HI-S	970	3000

For long-term simulations, 2016 weather was repeated each year to minimize potential confounding effects of inter-annual weather variability. The 2016 weather was representative of 30-year average temperatures and precipitation recorded at the nearby RTIA station [30]. Dates for irrigation, sowing, harvest, and tillage in 2016 were repeated throughout the long-term simulations. Especially for the high irrigation scenarios, plant growth decreased after a few years due to nitrogen (N) limitations, possibly due to excessive NO<sub>3</sub> leaching. To eliminate confounding effects of nutrient limitation, we used APEX's auto-fertilize function in scenarios where N stress exceeded 10 days per growing season. The scenarios enabled examination of the proportion of salt removed relative to the total inputs for the 15-year period.

#### 3. Results

#### 3.1. Calibration

Few calibrations run provided good results simultaneously for all output variables, but overall, simulated and measured values showed closest agreement for STL and LAI (Figure 2). Calibrated values of STX1 and Parm86 were much larger than their initial values (Supplemental Table S1). The initial value for STX1 was based on results from the greenhouse experiment, but it increased by a factor of 2.2 after calibration, resulting in a flatter salt stress curve. This flattening caused salt stress to be less sensitive to soil salinity as it deviated from the optimal value defined by STX2. Parm86 increased by a factor of  $1.6 \times 10^4$  compared to the model's default value, allowing salts to be transported upward much more easily.



**Figure 2.** Calibration results for crop variables: (**a**) Observed and simulated standing live biomass (STL) from germination to harvest in non-saline plot; error bars represent standard deviation (n = 3, except on July 12 n = 1); (**b**) Observed and simulated leaf area index (LAI) from germination to harvest in non-saline plot; error bars represent standard deviation (n = 3, except on July 12 n = 1); (**c**) Observed and simulated salt in quinoa biomass (USLT) from germination to harvest in non-saline plot; error bars represent standard deviation (n = 3, except on July 12 n = 1); (**c**) Observed and simulated salt in quinoa biomass (USLT) from germination to harvest in non-saline plot; error bars represent standard deviation (n = 3, except on July 12 n = 1).

After calibration, simulated STL on the harvest date exceeded the mean measured value by 26%, but the simulated value was still within the standard deviation of observations (Figure 2a). Simulated STL increased until harvest, but measured average biomass peaked around August 24 and stayed constant until the harvest date. Simulated LAI values followed the pattern of observed values, but underestimated LAI on the harvest date by 38% (Figure 2b).

While the calibrated model generally underestimated salt in plant biomass (USLT), the simulated biomass salt amount on the harvest date was within the standard deviation of the measured value (Figure 2c). Both observed and simulated biomass salt increased overall throughout the growing season, but changes in USLT were less gradual through time. All calibration runs had biases below -30% for USLT, indicating that salt in biomass was consistently underestimated, and the RMSE for USLT always exceeded 200 kg/ha. In contrast, bias values indicated that soil salinity (WSLT2) and soil water

content (SW2) at 10 cm were overestimated (Table 2; Figure 3a,b). Simulated soil salinity generally increased with irrigation and/or precipitation events, but simulated soil salinity appeared to be much more dynamic than measured (Figure 3a). During the irrigation season (June through September), the model simulated drier soils than measured at 10 cm depth. The final irrigation application occurred on September 22, after which simulated values were typically higher than measured.

Cal. Stage	Output Variable	Units	n	Observed Range	RMSE	<i>R</i> <sup>2</sup>
1	STL	t/ha	7	0.25-4.51	0.57	0.93
1	LAI		7	0.16-2.00	0.28	0.90
1	SW2	m/m	146	0.24-0.46	0.064	0.020
1	USLT	kg/ha	7	39.6-758.4	216.3	0.48
1	WSLT2	dS/m	146	0.44-1.55	2.91	0.60
2	STL	t/ha	7	0.25-4.51	0.70	0.93
2	LAI		7	0.16-2.00	0.26	0.90
2	SW2	m/m	146	0.24-0.46	0.065	0.016
2	USLT	kg/ha	7	39.6-758.4	291.0	0.23

**Table 2.** Statistics for the best set of metrics in each calibration stage. See Table S1 for abbreviation descriptions. n is number of observations.

Simulated salinity in the 0–1 cm layer (layer 1) responded even more strongly to water inputs than in the thicker second layer (1–19 cm; Figure 3c). Observed near-surface soil salinity, measured at least once a month in June, July, and August, did not exceed 25 dS/m in any of the plots, but simulated salinity in layer 1 exceeded 60 dS/m immediately after irrigation events. Following each peak, simulated salinity values quickly dropped to almost 0 dS/m as soil water percolated to the subsoil layer. The peaks of salinity in layer 2 indicate one to two days for the saline water to percolate from layer 1 to 2. Modeled salinity in layer 3 gradually declined until a heavy irrigation event on June 29 caused an increase in salinity from 0.3 to 1.8 dS/m.

Immediately following that increase, salinity in layer 4 increased from 1.3 dS/m to 2.0 dS/m. Modeled salinity in layers 5 and 6 remained relatively constant throughout the study as salt inputs were dampened by upper layers.

#### 3.2. 5-Year Scenarios

Long-term simulation results should be considered preliminary and are presented to demonstrate the utility of simulating plant-soil-water dynamics over time. Biomass production was predominantly affected by irrigation amount, while salinity only had a minor impact (i.e., LO-NS and LO-S produced similar biomass). In all scenarios, annual standing live biomass values stabilized after several years. Harvest day biomass in low irrigation scenarios (i.e., LO-NS and LO-S) stabilized at about 33% of the biomass in HI scenarios, and harvest day biomass in the MID scenarios was about 80% of HI scenario biomass. Model results indicated that biomass in low irrigation scenarios suffered from water stress more than two months per year for 11 of the 15 years.

Harvest day salt uptake amounts followed a similar pattern as biomass production. Low irrigation levels constrained biomass production and therefore also limited salt uptake, but more salt was taken up in MID and HI scenarios. At all irrigation levels, differences in salt uptake between saline and non-saline scenarios increased over time, with uptake being greater in saline scenarios. Differences in salt uptake between saline and non-saline scenarios were smallest at the lowest irrigation level. Annual salt uptake continued to increase over time for all saline scenarios, even as annual biomass remained constant. At the end of the 15th year, annual salt uptake was about 4.5 times greater in the HI-S scenario than in the LO-S scenario.

In all scenarios, salt accumulated in the root zone even when irrigation water salinity was low. The annual increase in root zone salinity was higher for the saline compared to non-saline scenarios. HI-S soils experienced the greatest salt input each year, resulting in an almost five-fold increase in salt content from the first to the last year of the simulation. For the five scenarios with lower salt input than the HI-S scenario, root zone salinity after 15 years was less than half that of the HI-S scenario. Simulated salt uptake relative to salt input was greatest for MID-NS, but uptake was less than 5% of salt inputs in all three saline scenarios (Supplemental Figure S1). Because there was some salt in irrigation water applied in 2016, even the non-saline MID-NS scenario resulted in the addition of 2283 kg salt/ha, exceeding the modeled crop removal rate by about four times.



**Figure 3.** Results for soil variables: (**a**) Observed and simulated daily soil salinity at 10 cm depth (WSLT2) in non-saline plot, along with moisture inputs from irrigation and precipitation; error bars represent standard deviation based on readings from two soil sensors; (**b**) Observed and simulated daily soil moisture at 10 cm depth (SW2) in non-saline plot, along with moisture inputs from irrigation and precipitation; error bars represent standard deviation based on readings from two soil sensors; (**c**) Simulated soil salinity (WSLT) in layer 1 (WSLT1) and layers 2–6 (WSLT2-6) of the non-saline plot in 2016. Note that salinity in the 0–1 cm layer is 10 times higher than shown in the graph.

#### 4. Discussion

We modified APEX to simulate quinoa, a halophytic crop, using empirically-based salt stress and salt uptake functions. Calibration of the modified APEX model using data from quinoa growth trials highlighted strengths and weaknesses of the model's salinity enhancements.

Simulated crop growth patterns were in general agreement with observed field data, indicating our salt stress function derived from the quinoa grown under greenhouse conditions was appropriate. However, other crops may show different response curves to salinity depending on the mechanism protecting plants against salt. For example, Adolf et al. [9] showed that salinity impacted biomass accumulation, salt accumulation, and other variables differentially among 14 quinoa varieties. Salinity responses of halophyte species examined by Vermue et al. [15] did not follow a symmetrical pattern. For instance, *C. maritima* biomass production increased from 0 to 9.8 dS/m, followed by a rapid decline in productivity above 9.8 dS/m. *S. dolichostachya* showed optimal productivity at 26 dS/m, with asymmetrical patterns of declining productivity above and below the optimal salinity [15].

Simulating plant salt uptake in APEX proved challenging. A good understanding of salt dynamics in the shallow root zone is critical for crop modeling, as plants typically extract a greater proportion of water (and thereby salt) from shallower depths [31]. Simulated biomass salt indicated irregular, discontinuous salt accumulation, and salt accumulation was minimal until two months after germination (Figure 2c). The low plant water demand (or root uptake) during the early stage of growth may have caused the slow start of salt uptake. Both biomass and plant salt concentration increased during the first five sampling events, but by the sixth and seventh sampling events, many senesced leaves had dropped to the ground, which was not accounted for in the simulated salt balance. Older leaves that senesced first likely accumulated greater concentrations of salt than young leaves [32,33]. In addition, by the sixth sampling event, water uptake, and consequently salt uptake, had most likely diminished in the field. The salt uptake function was based on vegetation samples collected at the end of the greenhouse experiment and further model development would benefit from additional data on plant salt concentrations throughout the growing season. Also, to better estimate crop salt content, salt concentrations in different parts of the biomass should be better quantified.

Quinoa's salt uptake dynamics may be different for other soil chemistries than those in this study. However, APEX is currently only capable of tracking total salinity. Due to the varying effects of different ions on plant salt uptake, ion-level modeling should be considered in future studies. Na<sup>+</sup> and  $Cl^-$  are widely known to be toxic to plants. Incorporating the impacts of other ions such as  $Ca^{2+}$  on the uptake of the major toxic ions will require additional study and model modification.

Since we did not have data beyond our experimental range, we were not able to verify plant salt concentrations beyond the soil salinity level of 12.4 dS/m (Figure 1). We note, however that plant biomass production shows a threshold behavior as soil salinity continues to increase. Given the large decrease in biomass production, but smaller increase in plant salt concentrations at higher soil salinity levels, overall total plant salt uptake decreases at higher salinity levels. Still, the plant salt concentration response curve may have resulted in an overestimate of salt uptake at higher soil salinities. The long-term scenario studies showed that salt removal by plants is a negligible part of the overall salt budget, so slight modifications of the plant salt concentration response curve would have had minimal impacts on the long-term salt budgets. Having data at higher soil salinity levels would improve accuracy of modeling the plant salt content. It is possible that the salt concentration response curve would display asymptotic behavior where, at high soil salt concentrations, plant salt concentrations will no longer increase but rather remain constant.

Reasonable simulation of hydrology is critical for proper representation of solute (e.g., salt) movement in soil. APEX captured dynamics associated with irrigation and precipitation events, but simulated and measured soil moisture levels at 10cm depth did not always agree (Figure 3b). This could have been because soil sensors for measured soil moisture and EC were not in plots used for crop growth monitoring, but in nearby locations. Plots with sensors had low vegetative cover due to lack of germination, so ET at sensor locations may have been different from ET at monitored plots, particularly during crop development stages when transpiration was high. Improved sensor placement at multiple depths, as well as more even irrigation application, may improve hydrologic calibration results in future studies. Including additional hydrology parameters in the sensitivity analysis may also lead

to the inclusion of additional parameters in the calibration. Changes in hydrologic parameter values would subsequently affect salt dynamics.

Despite similar patterns of soil moisture between modeled and field values, patterns in simulated soil salinity differed from those observed in the field (Figure 3a). Oscillations in salinity coincided with hydrologic events, but simulated fluctuations, particularly in the shallowest soil layer, were much larger than observed (Figure 3c). The 0–1 cm layer is especially vulnerable to salt accumulation, as evaporation is a key process occurring near the soil surface. The calibrated value of Parm86, which regulates upward salt movement by evaporation, was set at 16.058, but subsequent investigation with this value indicated that 1.0 might have been a more appropriate value that resulted in better estimates of soil salinity. Calibration was focused on simultaneously calibrating a subset of parameters affecting salt dynamics and crop growth, which may have led to selecting a higher value of Parm86. A more comprehensive calibration may have resulted in a better adjustment of Parm86 and a less dynamic behavior of salts in the soil.

Other studies have simulated quinoa (var. Titicaca) in Mediterranean climates with saline treatments using SALTMED [14,34,35], but they did not address root zone salinity dynamics and SALTMED does not account for crop salt uptake. Goodness-of-fit values for soil moisture, dry matter, and grain yield were generally better than in our study, particularly for soil moisture, which may reflect the smaller scale of the field plots in those studies as compared to ours, enabling better control of field irrigation volumes. In Kaya and Yazar [35],  $R^2$  for soil moisture at 0–30 cm was 0.88; in Pulvento et al. [34],  $R^2$  for soil moisture at 0–36 cm was 0.84; the study presented here had an  $R^2$  of 0.016 in the 1–19 cm layer. The maximum relative error for dry matter yield was 13.1% in Kaya and Yazar [35]. Yield and dry matter in Pulvento et al. [34] had less than an 8% difference from observed values, while in this study, simulated harvest day STL was 26% greater than observed.

After maturity, quinoa is harvested for its seed. Due to lack of production in the field, we focused on biomass rather than seed production for this study. We suspect that high temperatures contributed to the lack of field seed production as quinoa typically grows in cooler climates. Average high temperatures in Reno in July and August exceeded 32 °C. The effect of high temperatures on seed filling was not included in the model algorithms. Significant water stress should not have occurred at MSFL given that fields were frequently irrigated and soil moisture levels were above 27% throughout the growing season. The lack of seed filling may have affected late-season biomass and salt content. Future studies should focus on selecting crop varieties that are likely to thrive in the climate in which they are cultivated. In addition, Choukr-Allah et al. [11] noted in their studies that seed yield increased with greater nitrogen supply, so fertilization might produce better seed yields than in our study.

One advantage of the APEX model is that it allows for the assessment of long-term impacts of growing irrigated halophytes on crop productivity and soil salinity, as well as the relative effects of different agricultural management actions on crop growth, water quality impacts and salt removal. Our preliminary long-term simulation results should be interpreted with caution, but demonstrate the value of having the ability to look at plant-water-soil salt dynamics over the long term. Although quinoa is considered drought tolerant, simulations with reduced irrigation at our location during the growing season resulted in lower biomass. Simulations for the HI irrigation scenario required the addition of N fertilizer to minimize nutrient stress, indicating that supplemental fertilizer may be required even when water is not limiting growth. None of the long-term scenarios resulted in removal of significant amounts of salt from the soil because salt uptake was several orders of magnitude smaller than the amount of salt present in the root zone. More salt might be removed by increasing crop density or number of plantings per year, but this would require more water to maintain a high biomass production and it is unlikely that this increased salt uptake would offset an increased salt load associated with increased irrigation volume. Other halophytes such as Sesuvium portulacastrum L. (Aizoaceae) can be more effective than quinoa at salt uptake, capable of accumulating over 2500 kg/ha of Na<sup>+</sup> over 170 days [36]. However, plants considered in Rabhi et al. [36] were not crops, and thus lacked the additional benefit of food production offered by quinoa and many other halophytes.

Further improvements to APEX could enable evaluation of agricultural managements such as cover crop, residue management, and conservation tillage and their influence on soil salinity and TDS concentrations in groundwater and streamflow. In addition, trade-off analyses are needed to learn how these managements influence crop yield, nitrogen balances, carbon sequestration, and greenhouse gas emissions along with varying levels of salt removal. Irrigation management options should be carefully assessed, particularly in areas with limited good quality water [15]. The model approach should also be tested with experimental data that covers more than one growth season. Ultimately, applying the model to do feasibility assessments of remediating salt-contaminated land using halophytes instead of other engineering options would be of great interest among policy makers and engineers.

## 5. Conclusions

This study was an initial attempt at using APEX, a comprehensive watershed model, to simulate halophyte production alongside salt dynamics in the plant-soil-water system. Future model development should refine salt uptake improve parameters influencing salt movement in evaporation-influenced soil layers. Additional field data will help refine salt uptake algorithms and stress curve design. Preliminary long-term scenario simulations with different irrigation quantities and qualities indicated that irrigation water quality may have a cumulative impact on root zone soil salinity.

Halophytes can be highly productive in saline soils and may provide economic and environmental benefits, but our modeling results indicate that quinoa may not be effective for removing substantive amounts of salt from soil. With further improvement of salt dynamics, APEX can be useful for understanding salt dynamics and crop production for sustainable management options on marginal lands.

**Supplementary Materials:** The following are available online at http://www.mdpi.com/2073-4395/9/10/592/s1, Table S1: APEX input parameters relevant for this study [25]. Figure S1: Percentage of salt removed by quinoa relative to salt input via irrigation across 15 years. APEX salt source code is available at https://bitbucket.org/J9849/apex\_salt/src/master/ and model data are available in Goehring [37].

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#### Appendix A Greenhouse Experiment

Rainbow quinoa (Brightest Brilliant Rainbow from Wild Garden Seed, Oregon, USA) was seeded in 40.6 cm tall, 6.23 L pots using topsoil obtained from the field site (see Appendix B). In the greenhouse experiment, five soil salinities (2, 4, 6, 8, 12 dS/m) and four irrigation salinities (1, 2, 4, 6 dS/m) were employed to create 20 different treatment combinations. Each treatment was replicated five times. Salinity treatments were created using a mixture of 80% Na<sub>2</sub>SO<sub>4</sub> and 20% CaCl<sub>2</sub> by mass and soil salinity was measured using the saturated paste extract method [26]. Plants were watered every day or every other day and irrigation volumes were limited so that the saline solution would not drain from the pots. Irrigation volumes increased as plants grew to avoid water stress. Plant growth analysis measurements included leaf length and width, number of leaves, plant height, and number of branches on two plants per treatment. Plants were harvested prior to complete seed ripening. Leaf samples from the harvested plants were analyzed for plant salt concentration.

#### Appendix B Field Experiment

A field trial was conducted in 2016 at the University of Nevada, Reno, Main Station Field Lab (MSFL) in Reno, Nevada, USA (39°30' N, 119°77' W, elevation 1338 m AMSL). Soils belonged to the Truckee series (fine-loamy, mixed, superactive, mesic Fluvaquentic Haploxerolls). Soil salinities in the top 10 cm near the selected plots ranged from 0.6 to 1.8 dS/m, while salinities at 50–60 cm ranged from 0.5 to 4.2 dS/m. Rainbow quinoa was seeded during the last week of May 2016. We continuously measured soil moisture and salinity at selected plots at 10 cm and 40 cm depths using Decagon 5TE sensors. Surface (0–5 cm) salinity measurements were taken in all plots every two weeks using a Decagon 5TE probe connected to a hand-held datalogger.

The 10 m by 10 m plots were irrigated about once per week via hand line sprinklers. The fields were irrigated using treated wastewater having an average salinity of 420 mg/L [38] from the nearby Truckee Meadows Water Reclamation Facility (Figure A1). A total of 544 mm of irrigation water was applied with sprinklers from June through September. No fertilizer was applied at the MSFL field site.

Crop growth was monitored in one plot. Plant growth was monitored approximately every two weeks from early July through late September at MSFL according to protocols provided by J. Kiniry [39]. Light interception near the base of the plants was measured with a ceptometer in 0.25 m<sup>2</sup> quadrats. Aboveground biomass of plants within each quadrat was harvested to measure the area and mass of various plant parts and to analyze the dried biomass for nutrient and mineral (salt) content. Wet and dry weights were recorded, along with crop height and plant density data. Measurements and samples were collected in three quadrats in the plot during each sampling date.

Although quinoa biomass production was considerable, only a few seeds were produced, and as a result, plants were not harvested for seed. The theoretical harvest date for modeling purposes was set at September 26, 2016 based on observations of plant maturity and onset of seed production (122 days to harvest).



Figure A1. Schedule of irrigation, tillage, seeding, and theoretical harvest for 2016 field trials.

#### Appendix C Sensitivity Analysis

A sensitivity analysis was conducted to determine which parameters have the greatest influence on model output and reduce the number of parameters for calibration. The sensitivity analysis included parameters that could potentially have a direct effect on crop growth and salt movement dynamics or that had been identified by earlier work to be sensitive (Table S1; [28]).

Runs were completed using the model setup for 2016 at MSFL, with each parameter changed one at a time with the exception of BD and BDD, which were changed simultaneously. The model was run at 0%, 25%, 50%, 75%, and 100% of each parameter's range, resulting in a total of 80 runs. Three metrics were used to compare model run results to the observed STL, LAI, SW2, USLT, and WSLT2: root mean square error (RMSE),  $R^2$ , and bias. The preferred parameter set was chosen based on minimizing RMSE, maximizing  $R^2$ , and having a bias close to 0. A parameter was not considered sensitive if metrics (i.e., RMSE,  $R^2$ , and bias) were static upon changing that parameter's value.

## Sensitivity Analysis Results

STL, LAI, USLT, SM2, and WSLT2 were not sensitive to changes in UW, FC, Parm95, Parm61, and Parm38 as RMSE, R2, and bias values remained nearly constant upon changes of these parameters. As a result, these parameters were not included in the calibration process. Twelve other tested parameters (DMLA, BD, BDD, SAN, SIL, WOC, WA, SATC, STX1, STX2, ECND, and Parm86) were more sensitive because the RMSE, R2, or bias values for at least one of the output variables (STL, LAI, SW2, USLT, and WSLT2) varied significantly across the tested range. Based on field data, we had direct estimates for DMLA, BD, BDD, SAN, SIL, and WOC, so these parameters were also excluded as calibration parameters. Calibration therefore focused on the remaining parameters: WA, SATC, STX1, STX2, ECND, and Parm86.

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