SYSTEM DYNAMIC MODEL OF 1-DIMENSIONAL UNSATURATED WATER AND SOLUTE TRANSPORT FOR PREDICTING SALINITY STRESS IN CROPS

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Dedication

I would like to dedicate this thesis to my beloved wife and all my family members back home.

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Abstract

There is a complex non-linear system dynamic between the water and salt transport in the unsaturated vadose zone where the salt transport and accumulation affect the water fluxes and vice versa. In addition, factors such as precipitation, transpiration, water infiltration and solute transport in the unsaturated zone of subsurface soil further complicate the processes involved. We have developed a system dynamics model for simulating the one-dimensional unsaturated water and solute transport along with root water uptake in the vadose zone. The model uses finite difference method for solving Richard's equation with a sink term for water transport and root water uptake; and advection-diffusion equation for solute transport. The stock–flows for water and solute transport is discretized into different soil layers from top until it leaches out into an end stock. The root water uptake, water and solute transport are interconnected using physically based formulations and empirical assumptions. The model predicts the impact on root water uptake due to water and salinity stress as a function of matric and osmotic potential. The model's results were similar to the results from HYDRUS showing that the model is capable of predicting salinity and matric stress in crops and could be a useful tool for analyzing various geographical soil and crops.

El Paso county is located in the Chihuahua desert in Texas in an arid region with prolonged drought conditions. In order to evaluate the salt accumulation in the soil layers, we revisited a severe drought period in the history of El Paso with record low rainfall from 1947 to 1956. The system dynamic model was used to simulate water infiltration, solute transport and root water uptake for cotton and pecan crops with five different combinations of irrigation water. These waters had a common source as rainfall and two other sources of river and groundwater bringing an influx of solute into the system. Irrigation water with 100% groundwater predicted the highest salt concentration in the root zone in the range of 10 mg/cm^3 (15.6 dS/m) whereas 100% river

water predicted the lowest in the range of 2 mg/cm^3 (3 dS/m). The assessment of root water uptake for the first and last ten years of simulation period showed a reduction in crop yield for pecan and cotton by 44% and 88%, respectively.

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Section 1 – Development and Simulation of Model and Comparison with Hydrus

1.0 Introduction

Irrigation in arid and semi-arid region is complicated due to the presence of salinity in soil. Salinity is caused due to the presence of high concentration of salts in the soil that reduces the amount of available water for root water uptake by plants. The reduction in the root water uptake combined with effects of drought and other environment conditions limits the productivity of crop plants by 20% -50% of their maximum yield (Shrivastava & Kumar, 2015). A wide range of salinity stress management strategies are required to overcome such impacts of salinity on crop productivity. Keeping track of salinity in the soil and its associated reduction in root water uptake/ transpiration and crop productivity is the first step in understanding the salinity stress. Modeling the soil water movement, root water uptake and solute transport plays an important role in assessing the salinity stress and its related impacts on crops (Šimůnek, Suarez, & Sejna, 1996). In addition, evaporation and plant transpiration also plays an important role in the solution composition, water and solute distribution in subsurface conditions (Šimůnek et al., 1996).

The first approach to understand the complex relationship of salinity and crop growth was quantified by physically measuring the salt tolerance of various crops in a laboratory condition (Bernstein, 1956). This was followed with separate models on root water extraction using microscopic (Gardner, 1960; Molz, Fungaroli, Drake, & Remson, 1968) and macroscopic approaches (Dutt, Shaffer, & Moore, 1972) and salt transport (Bresler, 1973). The first combined model for soil water flow and root water extraction was proposed by (Nimah & Hanks, 1973). A comprehensive model combining soil water flow in unsaturated soil, root water extraction and solute transport was developed by Childs (1975) as an extension to the work by Nimah & Hanks (1973).

Later, various numerical models for the simulation of 1-dimensional water flow and solute transport were developed. These models were broadly categorized as steady-state and transient models. The steady state model, WATSUIT (Rhoades & Merrill, 1976) divides the root zone to four different zones vertically and assumes the root water extraction to be in the ratios of 40/30/20/10. It has a function of precipitation/ dissolution based on the presence or absence of $CaCO_3$ as an option. Whereas, the transient model simulates the continually changing soil water, salt effects on evapotranspiration, osmotic and matric effects on root water extraction, multi component major ion chemistry and transport, precipitation/dissolution, cation exchange, carbon dioxide - heat production and transportation. Some of the major transient models are ENVIRO-GRO (Pang & Letey, 1998), SALTMED (Ragab, 2002), SWAP (van Dam, 2000), UNSATCHEM (Šimůnek et al., 1996; D. L. Suarez & Šimůnek, 1997) and HYDRUS (Šimůnek, J., Huang, & van Genuchten, 1998; Šimůnek, J., van Genuchten, & Šejna, 2005; Šimůnek, M. Šejna, Saito, Sakai, & Genuchten, 2013; Vogel, Huang, & Zhang, 1996). The functionality of these models differs in the root water extraction component where SALTMED and ENVIRO – GRO uses an additive function whereas SWAP, HYDRUS and UNSATCHEM uses a multiplicative function while considering the osmotic and matric stress. Additionally, UNSATCHEM calculates the osmotic coefficient using the Pitzer equations from the major ion chemistry and incorporates a hydraulic reduction function due to salinity-sodicity interactions that further reduces the soil water flow. A comprehensive comparison of the simulated results on the yield of forage corn of these models has been done by Oster, Letey, Vaughan, Wu, & Qadir (2012). These models are developed using FORTRAN language and require an expertise personnel to integrate and modify various components as per user requirement. Whereas, system dynamic models provide the option for

participatory involvement from various stakeholders due to the simple, graphical and visual interactive platform of these models allowing easy modification and integration.

1.1 System Dynamic Approach

System dynamics is a graphical approach that can represent the dynamics of soil water flow, root water extraction and solute transport by numerically solving the finite difference equations at pre-determined timesteps. The system dynamic approach has been used for various hydrological and watershed studies (Keshta, Elshorbagy, & Carey, 2009; Ouyang, Xu, Leininger, & Zhang, 2016). A recent study using the system dynamic approach successfully simulated infiltration of water in the unsaturated zone using Darcy's equation showing the effectiveness of this approach (Huang, Elshorbagy, Barbour, Zettl, & Si, 2011). In this approach, the dynamic relation of the input, and its downward or upward movement is simulated based on the system's framework represented by equations and the feedback mechanism that is either reinforcing (positive feedback loop) or counteracting (negative feedback loop) (Huang et al., 2011). No studies were found that used the system dynamic approach to simulate the transient combined soil water flow, root water extraction and solute transport.

2.0 Model Overview

The objective of this study is to develop a system dynamic model simulating the transient soil water flow, root water extraction and solute transport in the vadose zone and quantify the effects of root water uptake under salinity and matric stress, and compare the results with a similar numerical model, HYDRUS. System dynamic models being graphical are easier to understand and visualize, particularly for non-expert stakeholders (e.g., growers). They use feedback loops to represent the systems that are reinforcing (positive feedback loop represented by "+") or counteracting (negative feedback loop represented by "-") as shown in Figure 1.1.

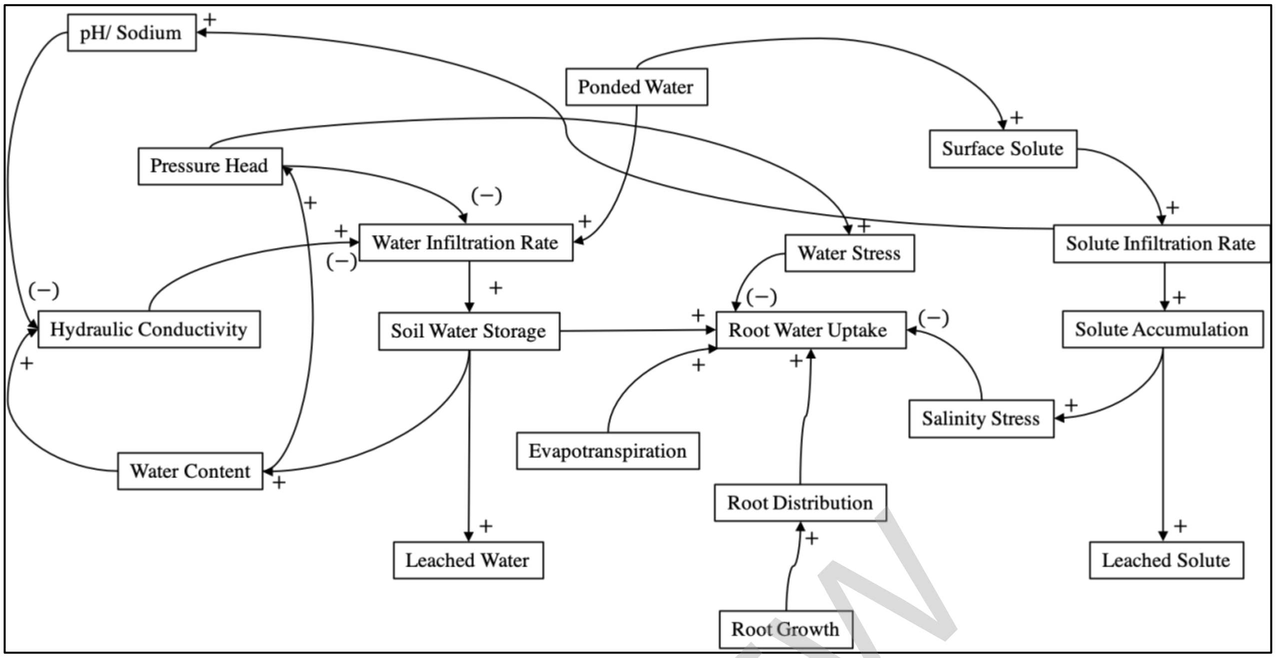

Figure 1. 1 – Casual loop diagram

During rainfall or irrigation event, the surface gets ponded with water. In due time, some water gets infiltrated and stored in the soil and; the rest leaches out. Once this system is in action, the loops formed by pressure head, hydraulic conductivity and water content becomes the driving force of the soil infiltration system. Increase in pressure head decreases the infiltration and increase in hydraulic conductivity increases infiltration, thus representing negative and positive feedback loops, respectively. When the roots of crop start to grow, it extracts water from the stored water in the soil. The extraction of water by roots increases the pressure head and in turn, builds up water stress on the crop reducing the crops ability to extract water from the soil layer, thus representing another negative feedback loop. Further, if the irrigation water or rain contains dissolved salt, it gets infiltrated into the soil and accumulates in the root zone. This accumulated salt will buildup salinity stress and sodacity of the soil. Salinity stress reduces the roots ability to extract water and; sodacity and pH reduces the hydraulic conductivity that in turn reduces the infiltration rate. This

is again represented by negative feedback loops. The system dynamic approach simulates these nonlinear, dynamic and complex relation between the systems using these feedback loops.

Further, system dynamic models have substantial educational and learning benefits for stakeholders compared to conventional numerical modeling. These models are easily editable by stakeholders to integrate any additional formulation or assumptions without prior knowledge of conventional programming languages. Also, there are methods to develop online web-based interface for system dynamic models and share them widely. Seeking participatory involvement from stakeholders was one of the key reasons for developing a system dynamic stock and flow-based model. Further other models such as HYDRUS does not simulate the effects of soil pH and clay swelling in soil water infiltration.

Soil is heterogenous in nature and a numerical solution of Richards equation is required for simulating the one-dimensional flow in unsaturated soil (Parissopoulos & Wheater, 1990). The system dynamic approach is used for numerically solving Richard's equation using finite difference method (Celia, Bouloutas, & Zarba, 1990). The unsaturated soil hydraulic properties are based on a set of closed-form equations (van Genuchten, 1980) and using the capillary model of Mualem (1976). Root water uptake is modeled using a sink term in Richard's equation that was first proposed by Feddes & Zaradny (1978) and later modified to include osmotic stress by van Genuchten (1987). Solute transport between multi soil layer is simulated by numerically solving the advection-diffusion equation for a non-reactive and non-interactive solute (Allan Freeze & Cherry, n.d.) using a finite difference method (Celia et al., 1990).

The model is developed using ISEE systems STELLA Architect software. A daily time step was used for all simulations. Due to the binary arithmetic that the computer uses, the time step between calculations, delta time (DT), in the model is set at 0.125 that falls in the sequence of

$(1/2)^n$, i.e., every 1/8th of a day , thus optimizing the computational speed and avoiding round-off errors (ISEE Exchange).

Figure 1.2 shows the icon based skeletal structure of the model as depicted in the software interface. The model contains rectangular blocks that are the stock variables representing the accumulation of water and solute in soil layers, and water in roots. The soil water infiltration and root water uptake rate, and solute transport flux is simulated using the flow variable symbolized by valves, between the stocks. Variables and equation leading to the formulation of these flow variables are formulated using converters, symbolized by circles. The converters are connected to the flow variables using connectors symbolized by a line and arrow at the end.

The soil layer is divided into three compartments of 30 cm, 30 cm and 40 cm each measured from the top adding up to 100 cm of soil column under simulation that covers most of the root zone for irrigated cotton and pecan crops. The rainfall, irrigation water, evapotranspiration, root growth, consumptive water use of crops and salt concentration for a pre-defined time frame is loaded to a converter as a csv or excel file. By defining the root growth, consumptive water use, salt tolerance and root distribution, the model can be used to simulate various annual and perennial crops and presently, the model is simulated for cotton and pecan.

The model has four sectors namely, “Soil Water Flow” (SWF) simulating the unsaturated water flow, “Solute Transport” (ST) simulating the transport of solute between layers, “Root Water Uptake” (RWU) simulating extraction of water by roots under matric and osmotic stress from each layer and “Hydraulic Reduction” (HR) simulating the salt stress on soil water flow; as shown in Appendix A1, A2, A3 and A4. All of the four sectors are interconnected based on various formulations and empirical relations. STELLA gives a user the option for partial simulation by selecting one or more of the four sectors to be run individually and/or combined.

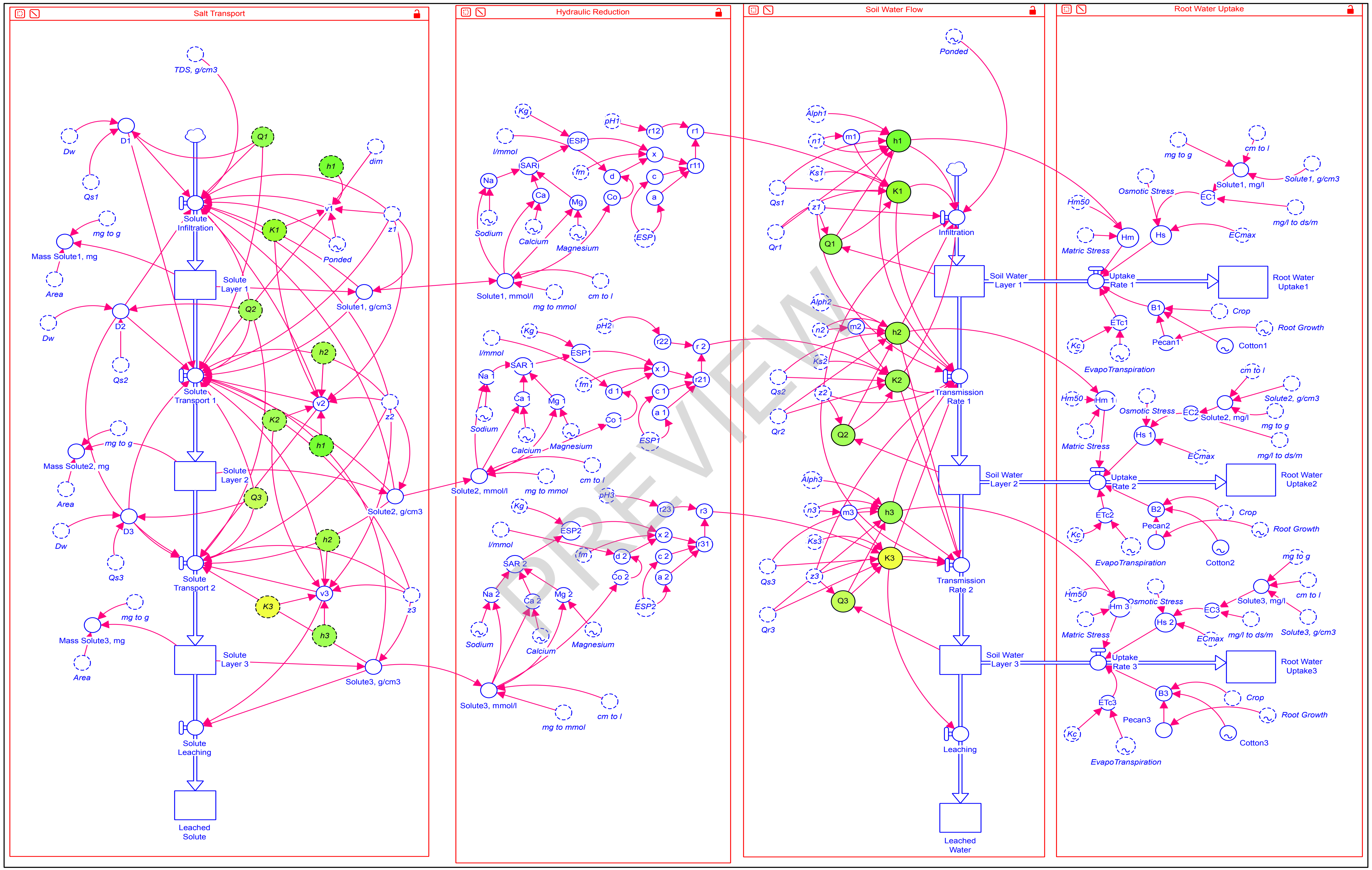

Figure 1. 2 – Icon based model skeletal structure as depicted in STELLA software

The building blocks within a selected sector is run dynamically keeping all other blocks static. This allows the user to set various combination of simulation based on the presence and absence of salt and matric stress.

The initial and top, and bottom boundary conditions for the SWF and ST sectors are assumed to be having a surface ponding due to rainfall and irrigation; and free drainage boundary conditions, respectively. The initial and top boundary condition is formulated using converters whereas the bottom boundary conditions is formulated using flow. The free drainage bottom boundary condition flows out to an end stock representing leached out solute and water from the soil.

3.0 Model Approach

The model is developed using the stock – flow – converter-based system dynamic approach to simulate the soil water movement, root water extraction and solute transport. The soil water flow in the unsaturated zone is considered as one-dimensional flow where the downward flow is driven by the hydraulic conductivity and pressure gradient of water. Coupled with the effects of solute buildup in the soil layer and root water extraction due to transpiration, the model simulates the water and solute movement and buildup in and below the root zone.

3.1 Soil Water Flow Sector (SWF)

The one-dimensional water flow in an unsaturated incompressible porous media is best described using the modified form of Richard's equation (Richards, 1952) formulated as:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[K\left(\frac{dh}{dz} + 1\right)\right] - S \qquad 1$$

where θ is the water content ($cm^3\ cm^{-3}$), h is the water pressure head/ capillary suction (cm), t is time (days), z is the depth of soil layer (cm) and S is the sink term ($cm^3\ cm^{-3} day^{-1}$) representing the root water extraction by the plants. The hydraulic conductivity and the capillary suction are

calculated using the Mualem (1976) and van Genuchten (1980) equations that was later modified to include the effects of soil chemical properties such as salt composition and *pH* (D. L. Suarez & Šimůnek, 1997):

$$\theta(h) = \theta_r + \frac{\theta_s - \theta_r}{(1 + |\alpha h|^n)^m} \qquad 2$$

and

$$rK(\theta) = \begin{cases} rK_s S_e^{1/2}\left[1 - \left(1 - S_e^{1/m}\right)^m\right]^2 & S_e < 1 \\ rK_s & S_e \geq 1 \end{cases} \qquad 3$$

respectively, where

$$m = 1 - 1/n \qquad n > 1 \qquad 4$$

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} \qquad 5$$

and where, θ_r and θ_s are the residual and saturated water content ($cm^3\ cm^{-3}$), respectively; K_s is the saturated hydraulic conductivity (cm/ day); S_e is the relative hydraulic conductivity; r is the hydraulic reduction function due to the soil chemical properties; and n and α (cm^{-1}) are the (van Genuchten, 1980) parameter of the soil water retention curve (SWRC).

3.1.1 Finite Difference Approximation

The conventional numerical solution of the Richard's equation considers the water balance of an infinitely small soil volume (Kroes, Van Dam, Groenendijk, Hendriks, & Jacobs, 2008) whereas in the system dynamic approach, the soil layer are considered as the stock variables and the rate of water movement is represented by the flow variables. Thus, an implicit backward finite difference method is used to solve the Richard's equation transforming it to a discretized form (Kroes et al., 2008):

$$\frac{\partial\theta}{\partial t} = \frac{1}{\Delta z_i}\left[K_{i-\frac{1}{2}}\left(\frac{h_{i-1} + h_i}{\frac{\Delta z_{i-1} + \Delta z_i}{2}} + 1\right) - K_{i+\frac{1}{2}}\left(\frac{h_i + h_{i+1}}{\frac{\Delta z_i + \Delta z_{i+1}}{2}} + 1\right)\right] - S_i \qquad 6$$

where subscript i represents the ith soil layer with values ranging from 1 to 3 and Δz_i is the soil compartment thickness. The sink term, S_i representing root water extraction is calculated as a separate stock – flow variable from each soil layer. Before defining the equations for flow between the soil layers, the boundary conditions should be defined for accurate simulation.

3.1.1.1 Boundary Conditions

The initial and top boundary condition is the flux of water entering the soil due to rainfall and irrigation represented by the converter 'Ponded depth' (*P*) (cm/day) given by:

$$P = Rainfall\ (cm/day) + Irrigation\ Water\ (cm/day) \qquad 7$$

For the initial condition, the data for daily rainfall and irrigation cycle is loaded as a datasheet in csv or Excel file. The bottom boundary condition is assumed to be free drainage condition represented by the converter '*Leaching*' equal to the hydraulic conductivity of the bottom and third layer (K_3). The drained or percolated water is collected to an end stock variable 'Leached Water' for tracking the amount of water drained out of the soil.

3.1.1.2 Water Flow Equations

The stock variable 'Soil Water Layer' (SWL) represent the water stored in the soil layers and therefore, the flow equations are multiplied by the soil compartment thickness, Δz_i.

In a flux controlled top boundary condition, the flow equation from the surface layer to the stock variable '*SWL1*' representing the water storage in first layer of subsurface soil has the term $K_{i-\frac{1}{2}}\left(\frac{h_{i-1}+h_i}{\frac{\Delta z_{i-1}+\Delta z_i}{2}}+1\right)$ replaced by flux of water entering the soil, *P*. The flow variable 'Infiltration' (I) (cm/day) representing this flow is given by:

$$I = P - \left[\frac{K_1+K_2}{2}\left(\frac{h_1-h_2}{\frac{z_1+z_2}{2}}+1\right)\right] \qquad 8$$