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USING SYSTEM DYNAMICS TO MODEL CESIUM PARTITIONING IN THE RHIZOSPHERE

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Running head: System Dynamics to Model Cs Partitioning in the Rhizosphere

ABSTRACT:

System Dynamics modeling is used to predict cesium (Cs) partitioning between bound, aqueous, and phytoextracted phases in the rhizosphere. The model categorizes processes that impact Cs fate into six sub-models. A seventh sub-model describes Cs flux between the three phases. Functional relationships and parametric values were developed based on literature, field, and laboratory data. Sensitivity analyses were conducted to evaluate the effects of root exudates on Cs partitioning, and the effects of root density, aerial plant density, potassium requirement/concentration, sodium concentration, and moisture content on root exudates and Cs partitioning. An increase in root exudate concentration results in a decrease in the bound Cs concentration and increase in the aqueous and phytoextracted Cs concentrations. Although the other parameters affect Cs partitioning partly according to how they affect root exudates, the comprehensive nature of the system complicates the overall effect.

INTRODUCTION

Radiocesium (particularly ^{137}Cs) is a common contaminant worldwide and one of the most common contaminants found at Department of Energy (DOE) sites (DART, 1999). Heavy metals and radionuclides are often detected as soil contaminants that threaten our natural resources. Radionuclides are of particular concern due to their ecological and human health risks that exist even when such contaminants do not come into direct contact with receptors. Typical treatment approaches include soil excavation and capping to minimize surface exposure and leaching into groundwater. However, such methods are expensive and do not extract the contaminants from the soil. Remediation of ^{137}Cs-contaminated soil is especially challenging because Cs selectively binds to mineral edge sites and within the soil matrix. Therefore, its release from the soil, and thus more effective remedial options, potentially requires the breakdown of the soil minerals.

It is envisioned that the biological and chemical effects of the plant root system can promote release and capture of Cs. In typical soil environments, Cs is partitioned in the pore fluid and on the soil solids. However, the presence of the plant roots in the rhizosphere, the zone where soil and roots interface, creates an additional sink for Cs. Accordingly, the partitioning between the three primary Cs pools: bound, aqueous, and phytoextracted, must be considered for proper evaluation of Cs fate in the rhizosphere.

Many of the mechanisms controlling the fate of inorganic compounds in the rhizosphere have been extensively studied and reported (e.g., Alloway, 1990). These mechanisms depend on concentrations and speciation of the metal in soil solution, as well as complex factors influencing the biological dynamics of the system. The primary areas affecting the partitioning of inorganic compounds may be categorized as geochemistry, geophysical factors, root and total plant morphology, microbial activity, nutrients, and root exudates. Of these factors, many have not yet been examined for Cs and particular plant systems, nor have the interactions of these factors been studied. Although extensive research has revealed innumerable effects within and between these areas, the scope of this current work is limited to developing an integrated comprehensive model for Cs solubilization in the rhizosphere.

SOLUTION PROCEDURE

Siegel *et al.* (2003) presented the preliminary formulation of this comprehensive model, which is implemented using Systems Thinking, integrating the relationships between the factors affecting Cs fate. The model categorizes the processes into six sub-models as defined by the primary areas affecting Cs partitioning. A seventh sub-model (Cs fate) relates the concentrations of the three specific forms of Cs: bound (Cs_b), aqueous (Cs_a), and phytoextracted (Cs_p). The overview of the model, including the interaction of the sub-models, is illustrated in Figure 1.

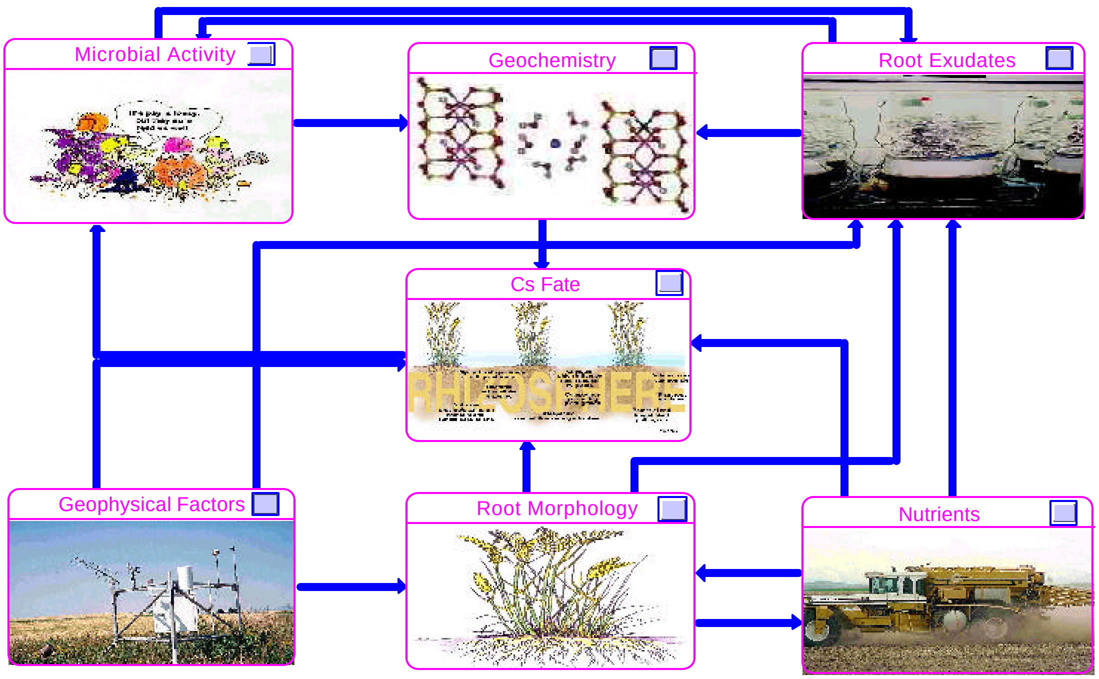

Figure 1: Schematic overview of model

Finite difference methods are used in the Stella® Research 6.0 software package (High Performance Systems, Inc., Hanover, NH) to numerically solve the system of differential equations that comprise the model. The software performs numerical integration according to one of three explicit methods (Euler's method, second-order Runge-Kutta, and fourth-order Runge-Kutta). Although each method provides similar output, Euler's method requires the least computing time and therefore has been applied to this model.

Integration error, i.e., the difference between the analytical and numerical solutions, may be a concern if delta time (DT) is too large. As DT approaches zero, the approximation approaches the analytical solution, where integration error is on the order of DT^2. However, this also increases the number of calculations to run the model. Therefore, choosing the appropriate DT requires a compromise between accuracy and speed. An acceptable difference (chosen to be less than 5% for this model) between the output with the DT and the output from re-running the model with 0.5·DT indicates that DT is adequate. Since this model describes a relatively slow process (on the order of days for Cs to change form), DT has been assigned to be 0.04 day, i.e., 25 simulations per day. Simulations for several conditions were tested with DT = 0.04 day and 0.5·DT, i.e., 0.02 day. The calculated concentrations for each partition and time were within 5% of each other. Therefore, DT = 0.04 day is indeed adequate.

DEVELOPMENT OF MODEL CODE

Functional relationships within and between the sub-models may be constants, equations, tabular input, or graphical interpretations of a relationship. Definitions of each functional relationship are based on literature, field characterization, and hypothesis-driven laboratory experimental data. Fluxes between accumulating variables derive directly from the mass balance and accompanying relationships.

The solutions for fluxes within the Cs fate sub-model, which is the crux of the comprehensive model, are presented here to demonstrate their derivation. $Flow_{sol}$, i.e., the flux between the bound phase and the aqueous phase and $Flow_{phy}$, i.e., the flux between the aqueous phase and the phytoextracted phase, shown in Figure 2, are based on the change in Cs_a with each discrete time step (Equation 1):

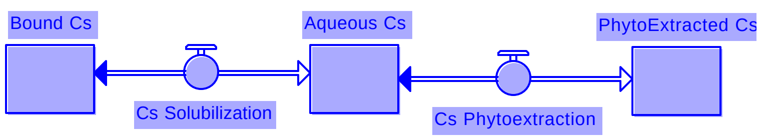

Figure 2: Cs partitioning

$$[1]\quad \frac{\Delta Cs_a}{\Delta t} = Flow_{sol} - Flow_{phy}$$

where

$$[2]\quad Flow_{sol} = \frac{\Delta Cs_{a-sol}}{\Delta t} = \frac{\dfrac{Cs_{EQ}(t)}{(1+K_{ND})} - Cs_a(t-\Delta t)}{\Delta t}$$

$$[3]\ Flow_{phy} = \frac{\Delta Cs_{a-phy}}{\Delta t} = \frac{CF_{ND} \cdot Flow_{sol} - Cs_p \cdot k_{release}}{1 + K_{ND} + CF_{ND}}$$

where Cs_{EQ} is the equilibrated Cs, K_{ND} is the non-dimensional adsorption relationship between the concentrations in the exchangeable and aqueous phases, CF_{ND} is the non-dimensional concentration factor, $k_{release}$, is the release of phytoextracted Cs back into the aqueous pool due to the decay of plant biomass, and Δ indicates that the changes are discrete approximations of the partial derivatives with time. Equation 3 indicates that as CF_{ND} increases, $Flow_{phy}$ approaches $Flow_{sol}$.

The change in Cs_{EQ} with time, which is required to solve $Flow_{sol}$, is determined according to the definitions of Cs_{EQ} and $Flow_{phy}$, (Equation 4).

$$[4]\ \frac{\Delta Cs_{EQ}}{\Delta t} = -\frac{\Delta Cs_i}{\Delta t} - Flow_{phy} \cdot (1 + K_{ND})$$

The change in K_{ND} with time is:

$$[5]\ \frac{\Delta K_{ND}}{\Delta t} = \frac{(K_{ND})_{t=0} \cdot F_C \cdot F_L \cdot F_{Ch} \cdot F_{pH} - K_{ND}}{\Delta t}$$

where F_C, F_L, F_{Ch} and F_{pH} are multiplicative factors adjusting K_{ND} due to competing cations, exudate ligands, microbial chelators, and pH, respectively.

The release of Cs from the mineral interlayers is:

$$[6]\quad \frac{\Delta Cs_i}{\Delta t} = \left(\frac{\Delta Cs_i}{\Delta t}\right)_D \cdot \left(1 + \frac{\left(\frac{\Delta Cs_i}{\Delta t}\right)_L}{\left(\frac{\Delta Cs_i}{\Delta t}\right)_D} : + \frac{\left(\frac{\Delta Cs_i}{\Delta t}\right)_{Ch}}{\left(\frac{\Delta Cs_i}{\Delta t}\right)_D} + \frac{\left(\frac{\Delta Cs_i}{\Delta t}\right)_{pH}}{\left(\frac{\Delta Cs_i}{\Delta t}\right)_D}\right)$$

where $\Delta Cs_i/\Delta t$ is the release of interlayer Cs with respect to time. Equation 6 indicates that the total $\Delta Cs_i/\Delta t$ is a function of the rate of release due to diffusion $(\Delta Cs_i/\Delta t)_D$ and the promoted releases rates, i.e., release due to ligands, chelators, and pH ($(\Delta Cs_i/\Delta t)_L$, $(\Delta Cs_i/\Delta t)_{Ch}$, and $(\Delta Cs_i/\Delta t)_{pH}$, respectively).

Equilibrium according to K_{ND} between the total bound and aqueous pools suggests that 100% of the bound pool is exchangeable, thus indicating a depletion of interlayer Cs. The model code reflects the depletion as the system approaches equilibrium as a multiplicative factor (F_e), which ranges from 0 to 1 in an assumed exponential relationship. If the ratio of the total bound concentration to the aqueous concentration is far from equilibrium, i.e., greater than $2 \cdot K_{ND}$, then the multiplier is 1 and $Cs_i/\ t$ as given by Equation 6 will occur. Otherwise, as the ratio approaches equilibrium, F_e reduces the rate of release until it is zero.

Solving numerically, Cs_a, Cs_b, and Cs_p at time t are:

$$[7]\ Cs_a(t) = Cs_a(t-\Delta t) + (Flow_{sol} - Flow_{phy}) \cdot \Delta t$$

$$[8]\ Cs_b(t) = Cs_b(t-\Delta t) - Flow_{sol} \cdot \Delta t$$

$$[9]\ Cs_p(t) = Cs_p(t-\Delta t) + Flow_{phy} \cdot \Delta t$$

PRESENTATION OF MODEL AND ITS COMPLEXITY

Figures 3 through 9 present the Cs fate, root exudate, and geochemistry sub-models, which illustrate that factors from each sub-model directly and indirectly affect the fluxes of Cs between the bound and aqueous phases and between the aqueous and phytoextracted phases. Table 1 lists the model parameters. The cockpit (Figure 10) is where key simulation input may be easily manipulated and simulation output is viewed.

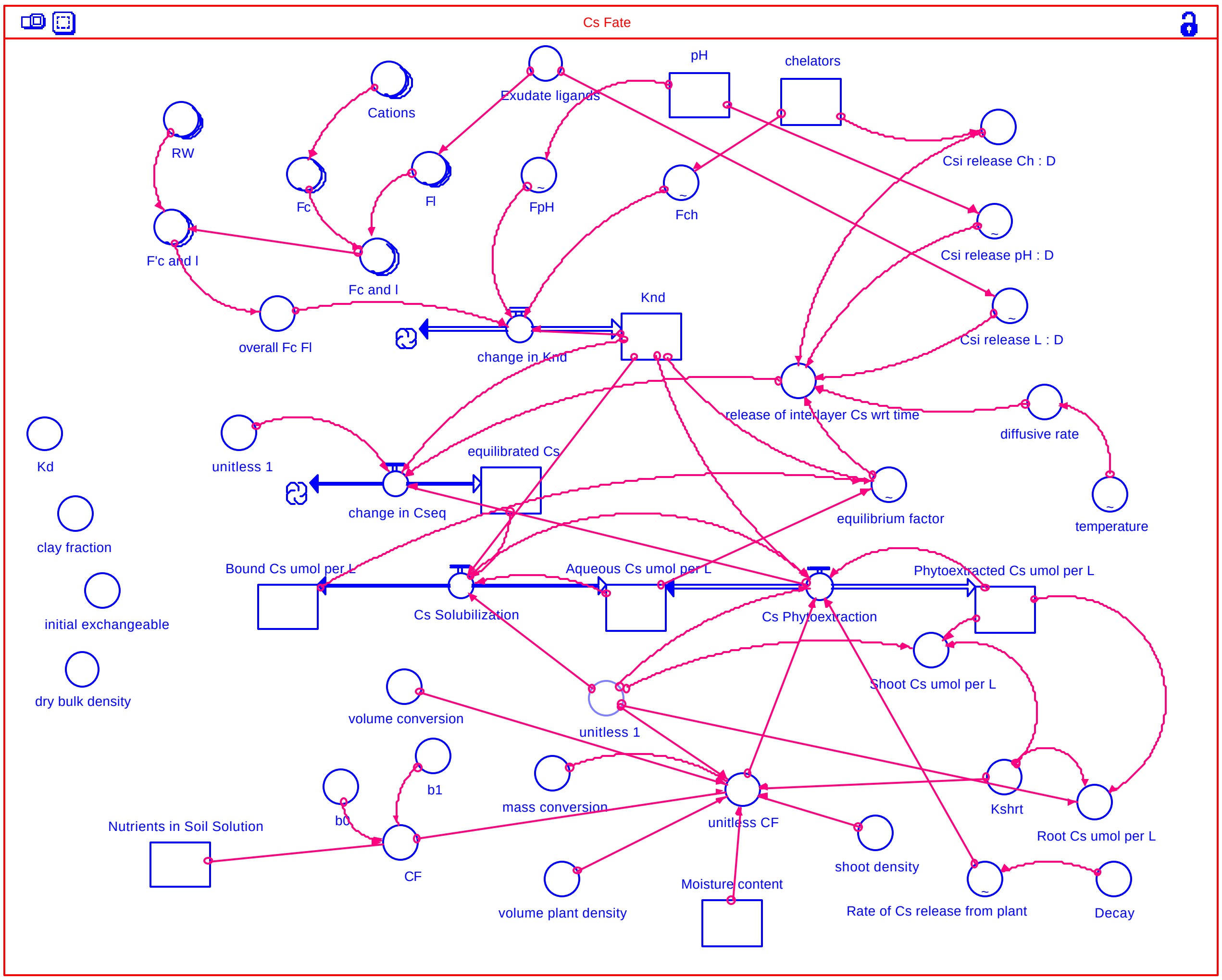

Figure 3: Cs fate sub-model. Multiple factors affect $\Delta Cs_i/\Delta t$, K_{ND}, and CF_{ND}, which affect Cs partitioning between Cs_b, Cs_a, and Cs_p.

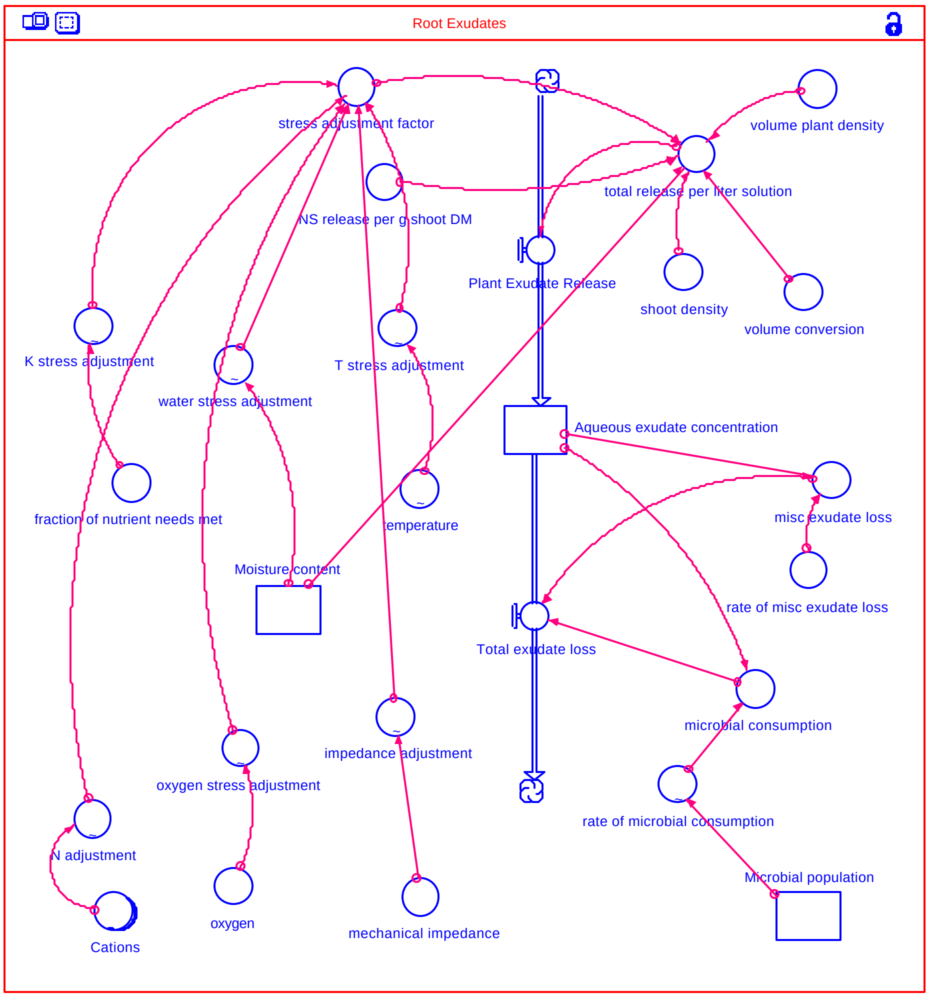

Figure 4: Root exudate sub-model. Environmental stressors influence exudate influx. Microbial consumption and miscellaneous loss determine exudate outflux.

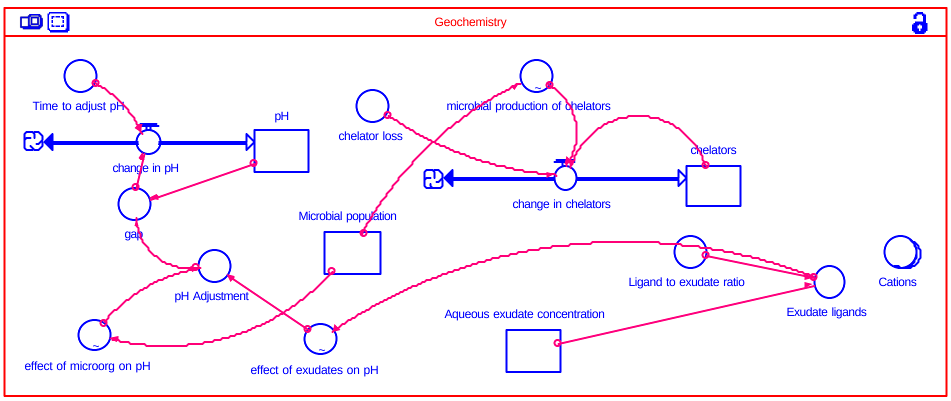

Figure 5: Geochemistry sub-model. Exudates influence the concentration of ligands and pH. Microorganisms influence the concentration of microbial chelators and pH.

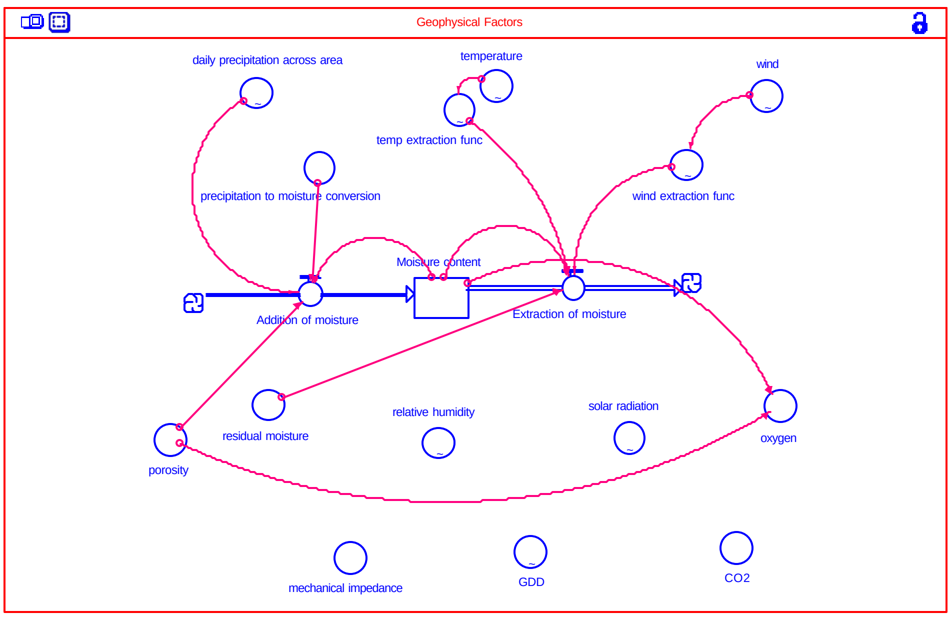

Figure 6: Geophysical factors sub-model. Defines meteorological and geophysical data.

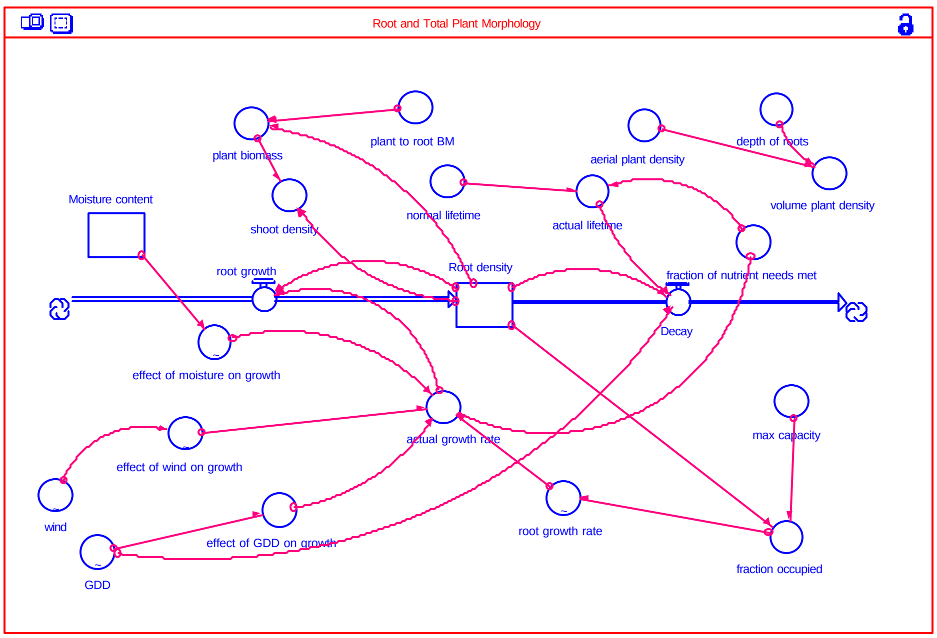

Figure 7: Root and Total Plant Morphology. Multiple factors influence growth and decay of plants.

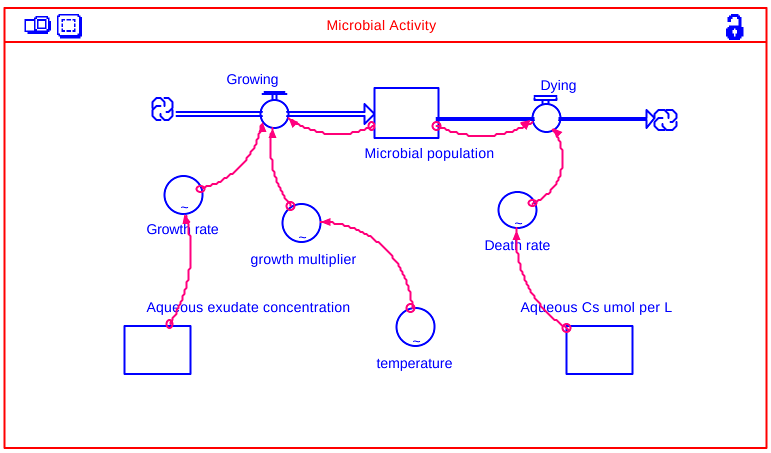

Figure 8: Microbial activity sub-model. The microbial population is a function of its growth rate and death rate.

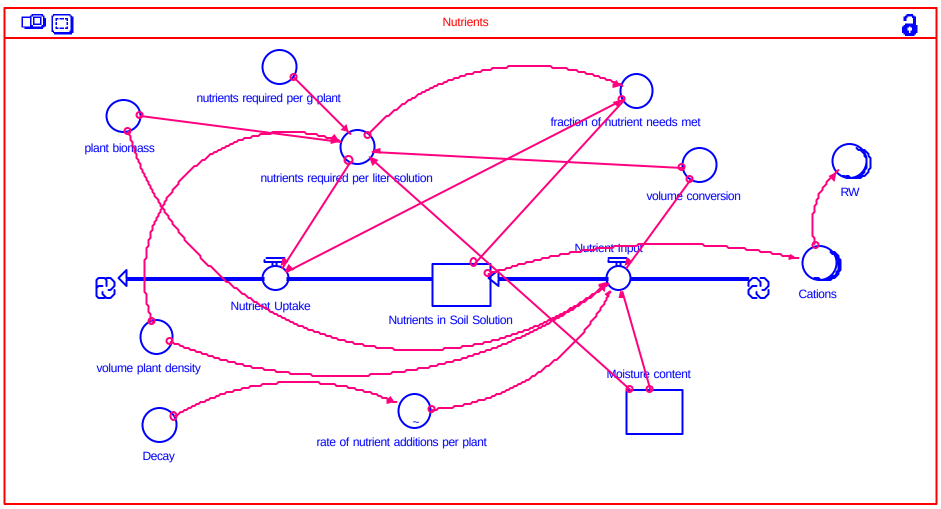

Figure 9: Nutrients sub-model. Nutrient uptake and input, affected by several factors, determine the nutrients in soil solution.

TABLE 1: MODEL PARAMETERS	
Stella Term	**Definition**
Stocks	
Bound Cs umol per L	Bound Cs (ì M), i.e., Cs_b
Aqueous Cs umol per L	Aqueous Cs (ì M) , i.e., Cs_a
Phytoextracted Cs umol per L	Phytoextracted Cs (ì M) , i.e., Cs_a
Equilibrated Cs	Equilibrated Cs (ì M), i.e., $Cs_{EQ} = Cs_a + Cs_e$
Knd	Non-dimensional adsorption relationship between the concentrations in the exchangeable and aqueous phases, i.e., $K_{ND} = \partial Cs_e/\partial Cs_a$
Aqueous exudate concentration	Exudate concentration (ì M), i.e., [E]
Moisture content	Volumetric water content, i.e., θ
Nutrients in Soil Solution	Sum of concentrations of potassium and nitrogen in solution
Microbial population	Number of microbes per mass of soil, i.e., MP
Root density	Root density, i.e., ρ_r
pH	PH
Chelators	Concentration of microbial chelators, i.e., [Ch]
Flows	
Cs Solubilization	Approximation of $\partial Cs_{a\text{-}sol}/\partial t$ by discrete DT, i.e., $Flow_{sol}$
Cs Phytoextraction	Approximation of $\partial Cs_{a\text{-}phy}/\partial t$ by discrete DT, i.e., $Flow_{phy}$
change in Cseq	Approximation of $\partial Cs_{EQ}/\partial t$ by discrete DT
Change in Knd	Approximation of $\partial K_{ND}/\partial t$ by discrete DT
Plant Exudate Release	Approximation of rate of exudate influx by discrete DT
Total exudate loss	Approximation of rate of exudate outflux by discrete DT
Change in chelators	Approximation of $\partial [Ch]/\partial t$ by discrete DT
Change in pH	Approximation of $\partial pH/\partial t$ by discrete DT
Root growth	Approximation of $\partial \rho_r/\partial t$ due to root growth by discrete DT
Decay	Approximation of $\partial \rho_r/\partial t$ due to root decay by discrete DT
Nutrient uptake	Approximation of $\partial [K^+]/\partial t$ due to nutrient uptake by plants by discrete DT
Nutrient input	Approximation of $\partial [K^+]/\partial t$ due to nutrient input by discrete DT
Growing	Approximation of $\partial MP/\partial t$ due to microbial growth by discrete DT

TABLE 1: MODEL PARAMETERS	
Stella Term	**Definition**
Dying	Approximation of ∂MP/∂t due to microbial death by discrete DT
Addition of moisture	Approximation of ∂θ/∂t due to precipitation by discrete DT
Extraction of moisture	Approximation of ∂θ/∂t due to extraction by discrete DT
Converters	
Release of interlayer Cs wrt time	Approximation of $\partial Cs_i/\partial t$ by discrete DT, i.e., $\Delta Cs_i/\Delta t$
Diffusive rate	$(\Delta Cs_i/\Delta t)_D$, i.e., $\Delta Cs_i/\Delta t$ due to diffusion
Csi release L : D	$(\Delta Cs_i/\Delta t)_L : (\Delta Cs_i/\Delta t)_D$, i.e., ratio of $\Delta Cs_i/\Delta t$ due to ligands to that due to diffusion
Csi release pH : D	$(\Delta Cs_i/\Delta t)_{pH} : (\Delta Cs_i/\Delta t)_D$, i.e., ratio of $\Delta Cs_i/\Delta t$ due to pH to that due to diffusion
Csi release Ch : D	$(\Delta Cs_i/\Delta t)_{Ch} : (\Delta Cs_i/\Delta t)_D$, i.e., ratio of $\Delta Cs_i/\Delta t$ due to microbial chelators to that due to diffusion
equilibrium factor	F_e
Fc, Fl, Fch, Fph	Multiplicative factors to adjust K_{ND} due to competing cations, exudate ligands, microbial chelators, and pH, i.e., F_C, F_L, F_{Ch} and F_{pH},
Fc and l	Combined effect of cations and ligands for each cation, i.e., $F_{C \cdot L}$
F’c and l	Weighted effect of each cation on K_{ND}, i.e., $F_{C \cdot L\text{-cation}}$
Overall Fc Fl	Overall effect of cations and ligands, (the sum of $F'_{C \cdot L}$ for each cation), i.e., $F_C \cdot F_L$
Kd	Linear isotherm constant relating exchangeable to aqueous Cs, i.e, K_d
Clay fraction	Fraction of the total soil that is assumed to contribute to K_{ND}, i.e., $Ö_K$
Initial exchangeable	Fraction of Cs_b that is exchangeable at time = 0, i.e., $Ö_E$
dry bulk density	Dry bulk density of the soil, i.e., ρ_b
b0, b1	Regression coefficients for empirical relationship for CF
CF	Concentration factor, CF, i.e., $\partial Cs_p/\partial Cs_a$
Volume conversion	Volumetric conversion factor, i.e., $conv_v$
Mass conversion	Mass conversion factor, i.e., $conv_m$
Unitless CF	Non-dimensional CF, i.e., CF_{ND}
Rate of Cs release from plant	Release rate of Cs_p into Cs_a due to plant decay, i.e., $k_{release}$
Kshrt	Ratio of the Cs pore fluid volumetric concentration in shoots to that in roots, i.e., K_{sh_rt}
Root Cs umol per L	Phytoextracted Cs (ìM) in roots

TABLE 1: MODEL PARAMETERS

Stella Term	**Definition**
Shoot Cs umol per L	Phytoextracted Cs (ìM) in shoots
Unitless_1	1, used to maintain unit consistency
Cations	Concentration of each cation, i.e., $[K^{+}]$, $[NH_4^{+}]$, $[Ca^{+2}]$, $[Mg^{+2}]$, and $[Na^{+2}]$
RW	Relative weight of cation with respect to total concentration of cations
Fraction of nutrient needs met	FNNM
Nutrients required per g plant	$[K^{+}]_{reqd}$
Nutrients required per liter solution	$[K^{+}]_{reqd}$ converted from per mass of plant to per volume of pore solution
Rate of nutrient additions per plant	Rate of input of nutrients to system
Plant biomass	Biomass of plant, i.e., BM
K stress adjustment	Adjustment to exudate release rate due to stress on plant system caused by $[K^{+}]$
N adjustment	Adjustment to exudate release rate due to stress on plant system caused by $[NH_4^{+}]$
Water stress adjustment	Adjustment to exudate release rate due to stress on plant system caused by θ
Oxygen stress adjustment	Adjustment to exudate release rate due to stress on plant system caused by O_2
Temperature stress adjustment	Adjustment to exudate release rate due to stress on plant system caused by T
Impedance adjustment	Adjustment to exudate release rate due to stress on plant system caused by mechanical impedance
NS release per g shoot	Exudate release rate under non-stress conditions
Stress adjustment factor	Adjustment to exudate release rate due to overall stress on plant system
Total release per liter solution	Pore fluid volumetric total influx of exudates
Rate of microbial consumption	Rate of exudate loss due to microbial consumption
Microbial consumption	Outflux of exudates due to microbial consumption
Rate of misc exudate loss	Rate of exudate loss due to miscellaneous loss
Misc exudate loss	Outflux of exudates due to miscellaneous loss
Death rate	Rate of death of microbial population
Growth multiplier	Multiplier effect of temperature on growth rate
Growth rate	Rate of growth of microbial population
Oxygen	Oxygen concentration in soil
Mechanical impedance	Mechanical impedance of plants
Effect of exudates on pH	pH due to exudate ligands
Effect of microorg on pH	pH due to microorganisms
Ph adjustment	Combined effect of exudate ligands and microorganisms on pH
Gap	Difference between pH and pH adjustment

TABLE 1: MODEL PARAMETERS	
Stella Term	**Definition**
Time to adjust pH	Time required to establish new pH
Ligand to exudate ratio	Ratio of ligands to exudates
Exudate ligands	Concentration of exudate ligands
Chelator loss	Outflux of microbial chelators from system
Microbial production of chelators	Influx of microbial chelators to system
Daily precipitation across area	
Precipitation to moisture conversion	
Porosity	
Temp extraction func	Effect of temperature on moisture extraction
Wind	Speed of wind
Wind extraction func	Effect of wind on moisture extraction
Residual moisture	Minimum moisture content
Relative humidity	
Solar radiation	
Oxygen	Oxygen concentration in soil
CO2	Carbon dioxide
GDD	Growing degree day
Mechanical impedance	Mechanical impedance of soil on plants (MI)
Plant to root BM	Ratio of plant biomass to root biomass
Normal lifetime	Typical lifetime of plant
Actual lifetime	Actual lifetime of plant
Aerial plant density	Number of plants per surface area of soil (ρ_p)
Depth of roots	Depth to which the roots extend
Volume plant density	Number of plants per volume of soil (ρ_{vol-p})
Max capacity	Maximum root density
Fraction occupied	Ratio of root density to maximum capacity
Root growth rate	
Actual growth rate	
Effect of GDD on growth	
Effect of wind on growth	
Effect of moisture on growth	
Shoot density	Mass of shoot per plant (ρ_s)

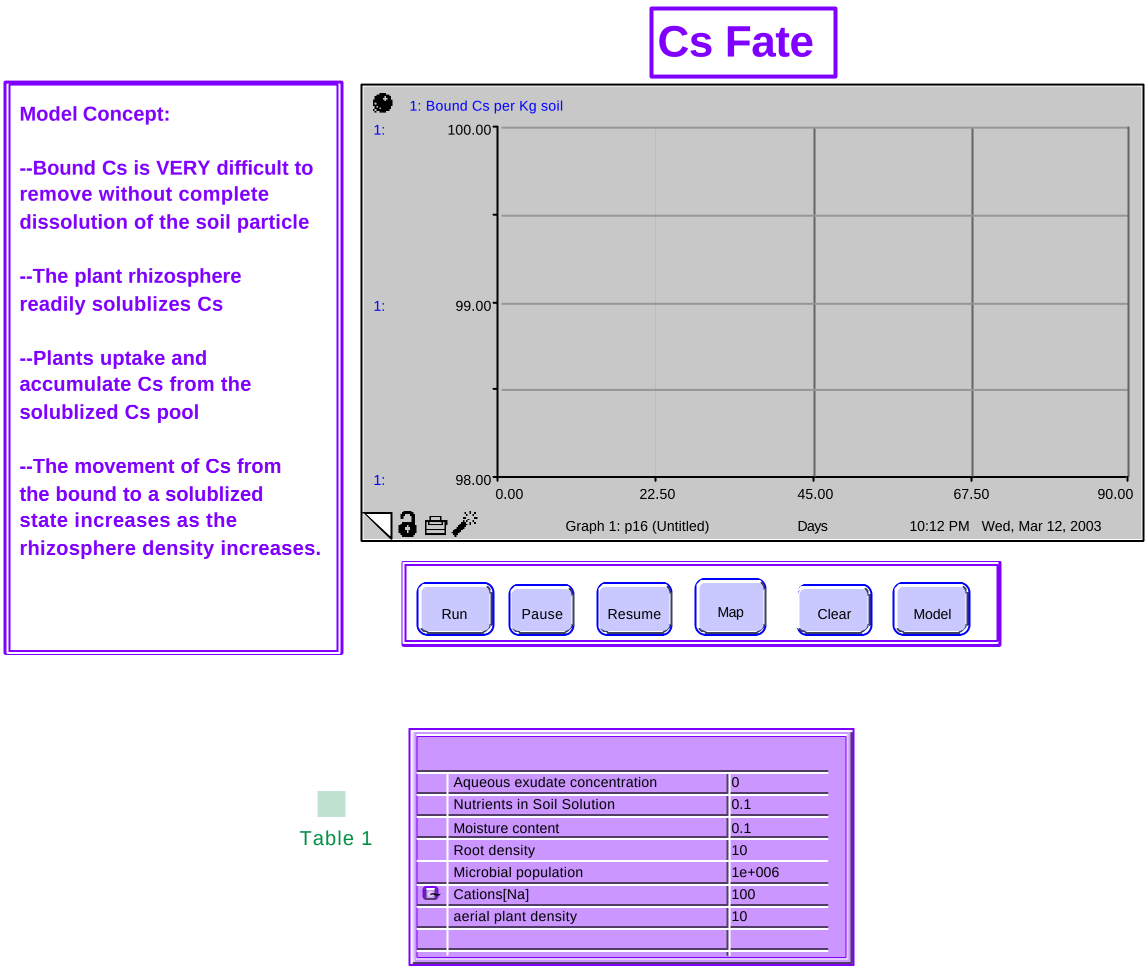

Figure 10: Model cockpit. Key simulation input may be easily manipulated and simulation output is viewed.

Complexity lies in the fact that many factors affect $\Delta Cs_i/\Delta t$, K_{ND}, and/or CF_{ND}, many of these factors affect each other, these relationships are typically non-linear, and the relationships may compete with each other. Several reinforcing and counteracting loops within and between each sub-model and connections between loops further complicate the overall effect on Cs partitioning. Figures 11 through 13 present examples of loops influencing the aqueous Cs concentrations. Figure 14 presents an example of a loop influencing the concentration of nutrients in solution and root density, which in turn may affect concentration of root exudates ([E]). The loop in figure 12, which includes [E], exemplifies the extent to which the interactions of processes are compounded.

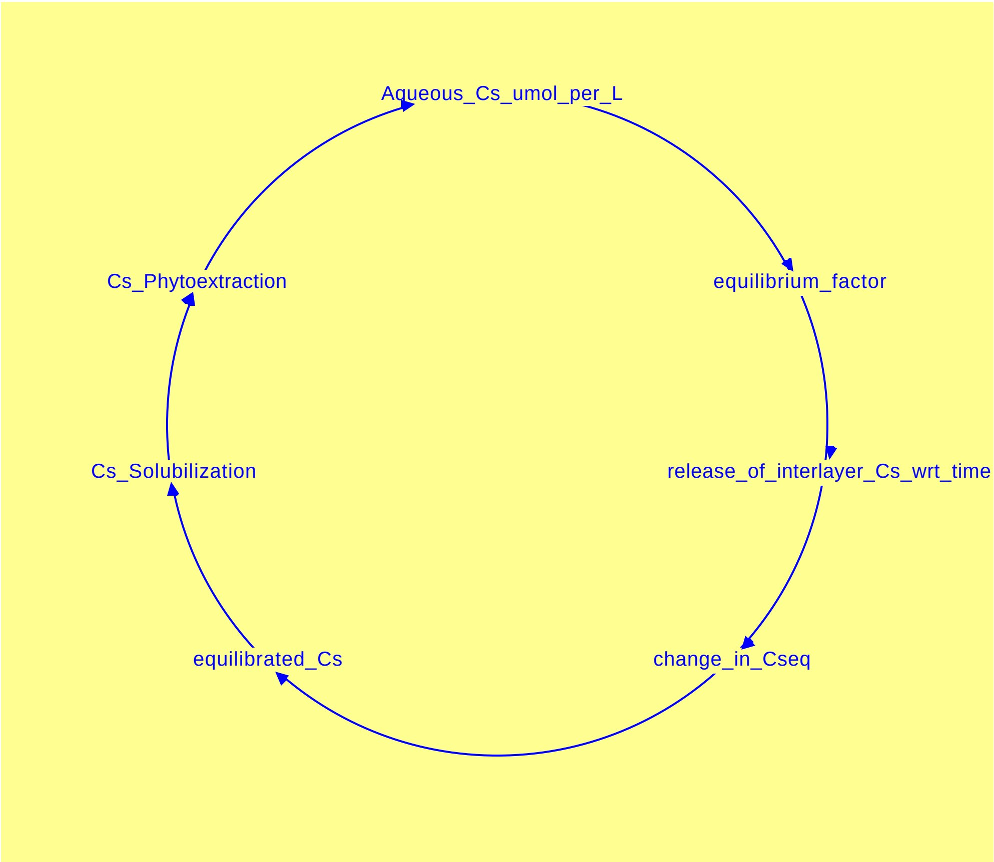

Figure 11: Example of loop influencing aqueous Cs concentration.

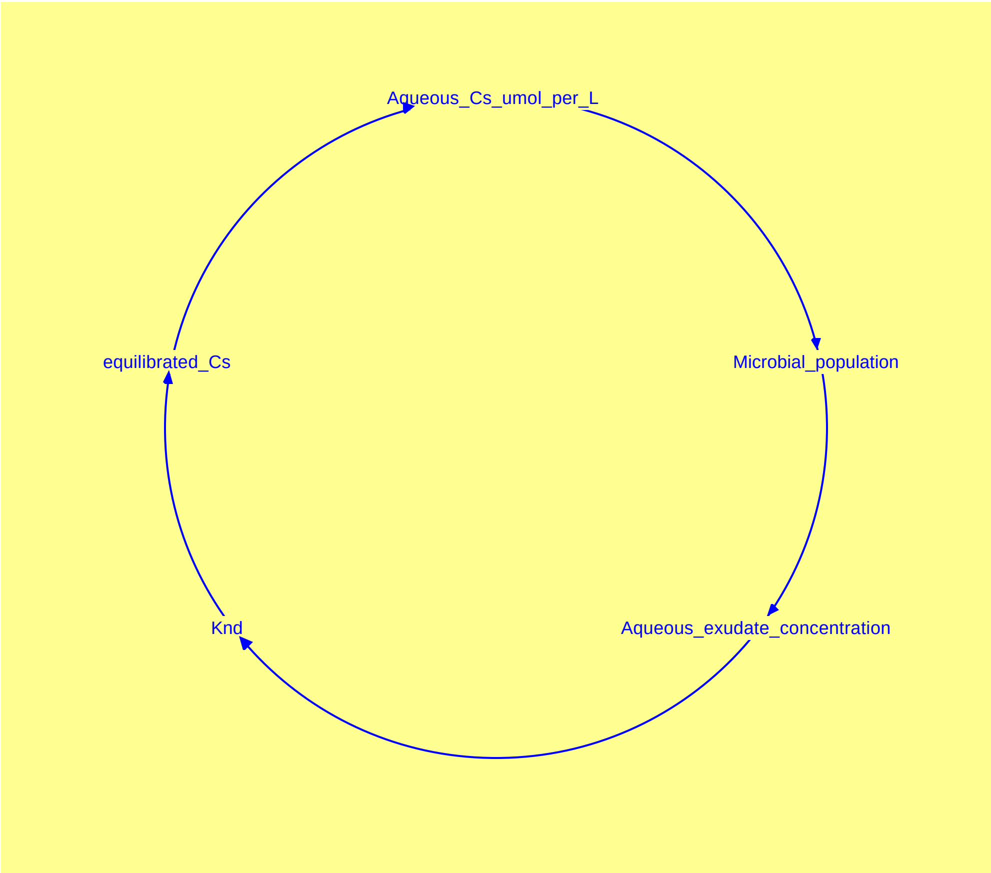

Figure 12: Example of loop influencing aqueous Cs concentration, which includes aqueous exudate concentration.

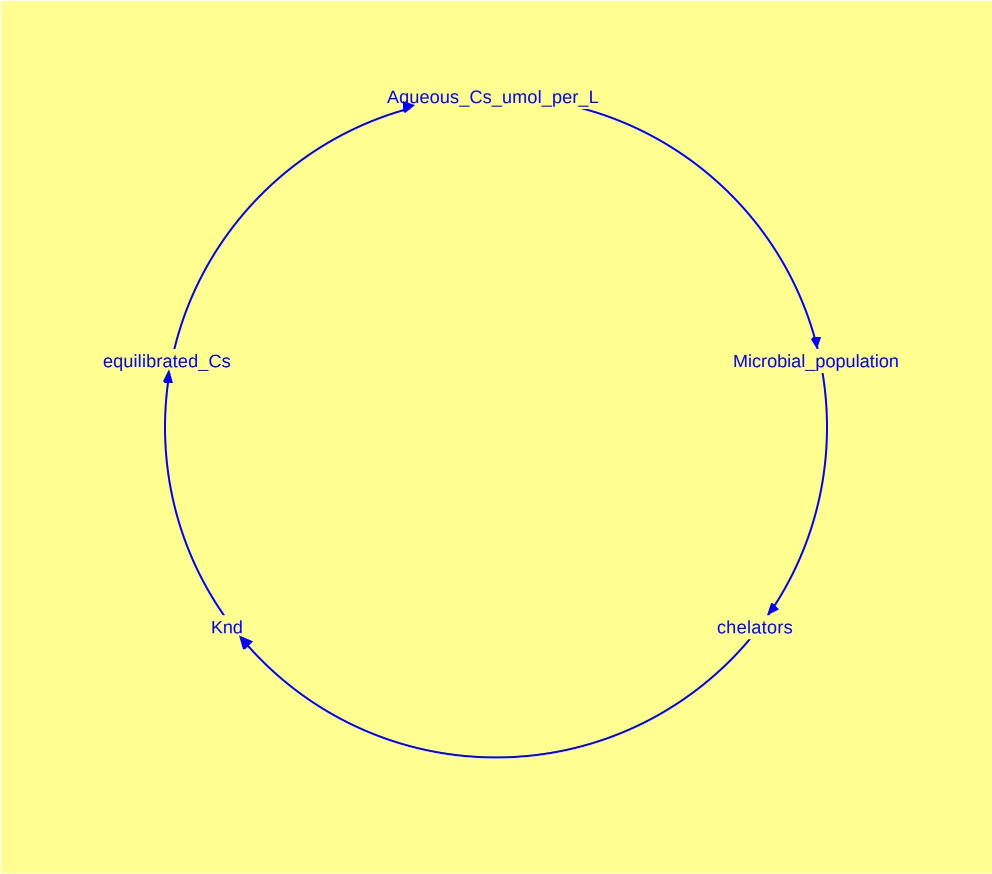

Figure 13: Example of loop influencing aqueous Cs concentration, which includes microbial population.

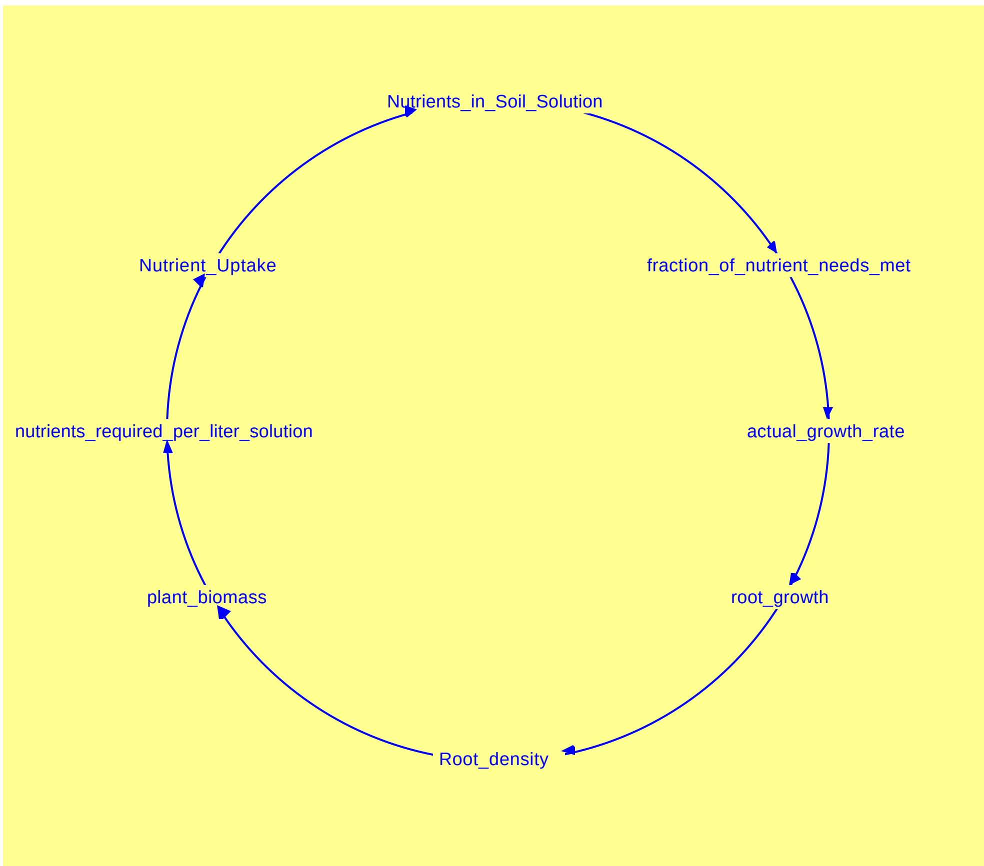

Figure 14: Example of loop influencing nutrients in solution and root density.

The primary focus of this research is currently to evaluate the effects of the [E] on Cs partitioning and to evaluate the effects of other parameters on [E]. An increase in [E] causes an increase in $\Delta Cs_i/\Delta t$ and a decrease in K_{ND}. Consequently, $Flow_{sol}$ and $Flow_{phy}$ both increase, resulting in a greater decrease of Cs_b and a greater increase of Cs_a and Cs_p. The functional relationships defining the multiplicative factor to adjust K_{ND} due to exudate ligands for each cation, i.e., $F_{L\text{-}cation}$, and the ratio of $\Delta Cs_i/\Delta t$ due to ligands to that due to diffusion, i.e., $(\Delta Cs_i/\Delta t)_L$: $(\Delta Cs_i/\Delta t)_D$, are responsible for the changes observed. The change in K_{ND} negatively relates exponentially to the ligand concentration. Thus, the increase in [L] from 0 to 0.1 mM produces a notable decrease in K_{ND}. On the other contrary, an increase in $(\Delta Cs_i/\Delta t)_L$ is not expected for [L] less than 1 mM (Drever and Stillings, 1997).

Root density (ρ_r), i.e., root mass per plant, and aerial plant density (ρ_p), i.e., plants per land surface area, affect Cs partitioning according to their effects on [E], and the consequential effects on $Flow_{sol}$ and $Flow_{phy}$, as well as their effects on CF_{ND}. An increase in ρ_r or ρ_p increases [E] by increasing the release of root exudates per liter of pore solution. Increasing ρ_r or ρ_p also increases [E] due to the resulting increase in the plant's nutrient needs, which decreases the fraction of nutrient needs met (FNNM), which imposes stress on the system, which increases the release of exudates per mass of plant. Furthermore, a denser root system or plant population increases CF_{ND}, which increases $Flow_{phy}$ and thus Cs_p. Although an increase in ρ_r or ρ_p yields an increase in the mass of phytoextracted Cs per volume of pore solution, the mass of plant is also increased with increasing root density. Therefore, the concentration per mass of plant may be less with a greater root density.

As indicated, Cs partitioning is also a function of the plant's nutrient requirements, particularly potassium required ($[K^+]_{reqd}$). As $[K^+]_{reqd}$ increases beyond the point where all needs are met, the FNNM decreases, causing a stress on the system and consequently an increase in the release of exudates. However, a change in requirements that does not reduce the nutrient needs met does not stress the system, and thus does not impart an influence on [E] nor on Cs partitioning. Increasing $[K]_{reqd}$ beyond the threshold requirement affects Cs partitioning in a qualitatively similar trend to those for increasing [E].

The potassium concentration in solution ($[K^+]$) also affects Cs partitioning due to its effects on FNNM as well as on its effects on CF_{ND}. Decreasing $[K^+]$ in solution instead of increasing $[K^+]_{reqd}$ likewise affects the FNNM, resulting in a potential increase in [E]. However, CF_{ND} is also a function of $[K^+]$, thereby complicating the effects. In that case, a decrease in $[K^+]$, which causes stress on the system and thus an increase in the release of exudates, also causes an exponential increase in CF_{ND}. Consequently, $Flow_{phy}$ approaches $Flow_{sol}$, i.e., the flux into the aqueous pool approaches the flux into the phytoextracted pool.

Besides potassium, other competing cations influence Cs partitioning, mainly due to their influence on K_{ND}. Typically, an increase in the concentration of a competing cation results in a decrease in K_{ND}. Such a decrease yields an increase in $Flow_{sol}$ and $Flow_{phy}$ and thus a greater decrease in Cs_b and greater increase in Cs_a and Cs_p.

The overall effect of moisture content (θ) on Cs partitioning is complicated by the fact that there are several individual effects. Dilution with increasing θ reduces [E]. An increase in θ may also reduce the level of moisture stress, thereby further decreasing [E]. However, an increase in θ to the point of flooding may increase oxygen stress, thereby increasing [E]. In each scenario, Cs partitioning is consequently affected accordingly. Furthermore, an increase in θ yields a decrease in K_{ND}, and consequently an increase in $Flow_{sol}$. Likewise, an increase in θ yields a decrease in CF_{ND}, resulting in a decrease in $Flow_{phy}$. The complexity expands when the effects of θ on the other variables discussed here are considered.

PARAMETER ESTIMATION AND SENSITIVITY ANALYSES

Hypothetical data, consistent with those presented in the literature, are used to estimate parametric values for which field characterization or experimental data are not available. Where practical, regression analysis on available data is used to determine the parametric values of each functional relationship.

Sensitivity analyses were conducted to isolate the effects of [E]. Elements outside the geochemistry and Cs fate sub-models are assumed constant. Figures 15a through 15c illustrate the influence that [E] (0, 1, 10, and 100 mM) has on Cs fate. It is clear that the rates of solubilization and phytoextraction are non-linearly related to the concentration of root exudates. Table 3 summarizes the effects of varying [E] on [L], K_{ND}, and $\Delta Cs_i/\Delta t$. The percentage increase for aqueous and phytoextracted Cs is greatest for [E] increasing from 1 to 10 mM, and the percentage decrease for bound Cs is greatest for [E] increasing 10 to 100 mM, although the percentages vary over several orders of magnitude.

TABLE 3: EFFECT OF CONSTANT [E] ON [L], K_{ND}, AND DCs_i/Dt				
[E] (mM)	**0**	**1**	**10**	**100**
[L] (mM)	0	0.1	1	10
K_{ND}	7575.10	283.50	4.86	4.67
$\Delta Cs_i/\Delta t$[1] (ì M·day^{-1})	6.48	6.48	12.96	330.48

[1] $\Delta Cs_i/\Delta t$ decreases according to F_e as Cs_b and Cs_a approach equilibrium.

Sensitivity analyses were also conducted to isolate the effects of root density (ρ_r), aerial plant density (ρ_p), potassium concentration ($[K^+]$), potassium required ($[K^+]_{reqd}$), sodium concentration ($[Na^+]$), and moisture content (θ) (Figures 16 through 21). For these analyses, the root exudates sub-model is run with the geochemistry and Cs fate sub-models to evaluate the effects of these parameters on [E] and Cs partitioning. Evaluations tested three values of each parameter, where the parameter variation covered the range of possible values. For ρ_p, $[K^+]_{reqd}$, $[K^+]$, and $[Na^+]$, parameters were varied by orders of magnitude. For ρ_r and θ, increasing by an order of magnitude is not realistic. Instead, evaluations tested the assumed minimum, typical, and maximum values for each parameter. Results demonstrate the complexity of the system as described in the previous section.

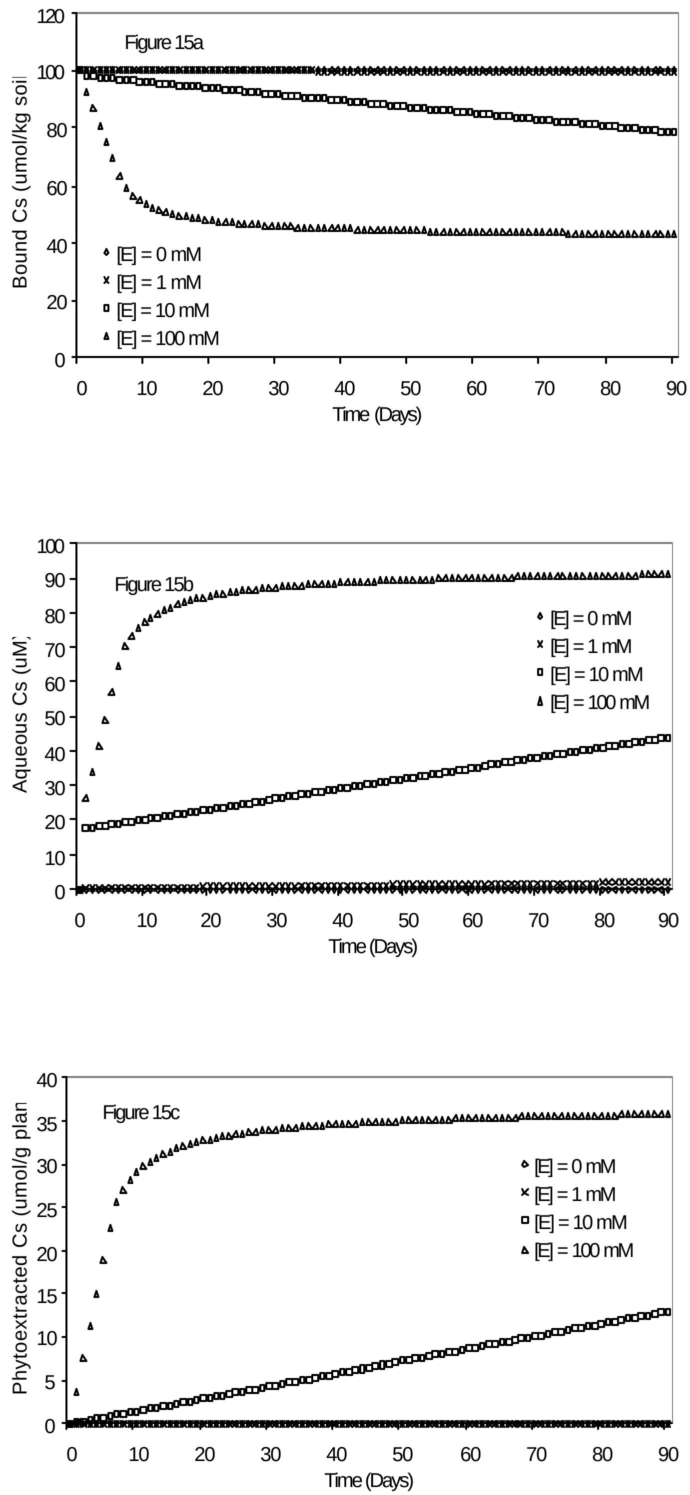

Figure 15. Effect of exudate concentration ([E]) on Cs partitioning.

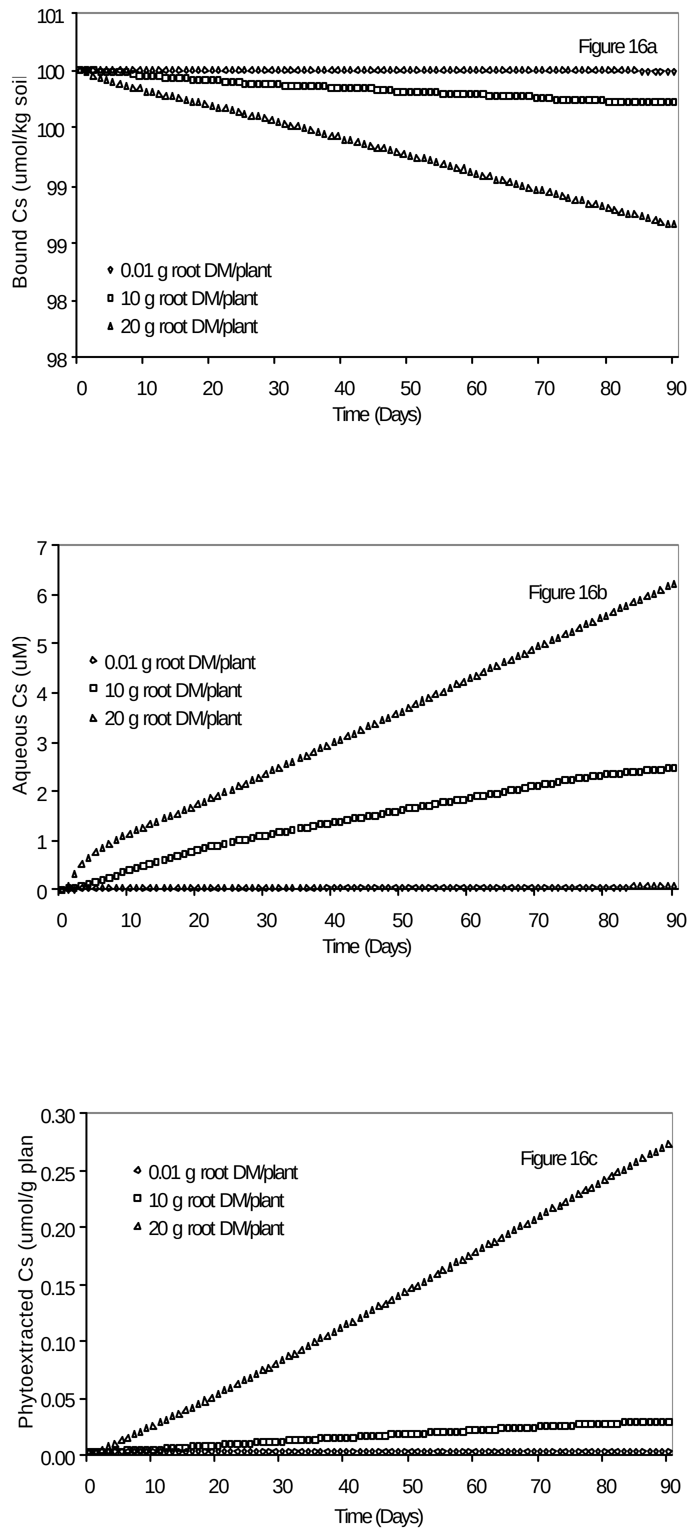

Figure 16. Effect of root density on Cs partitioning

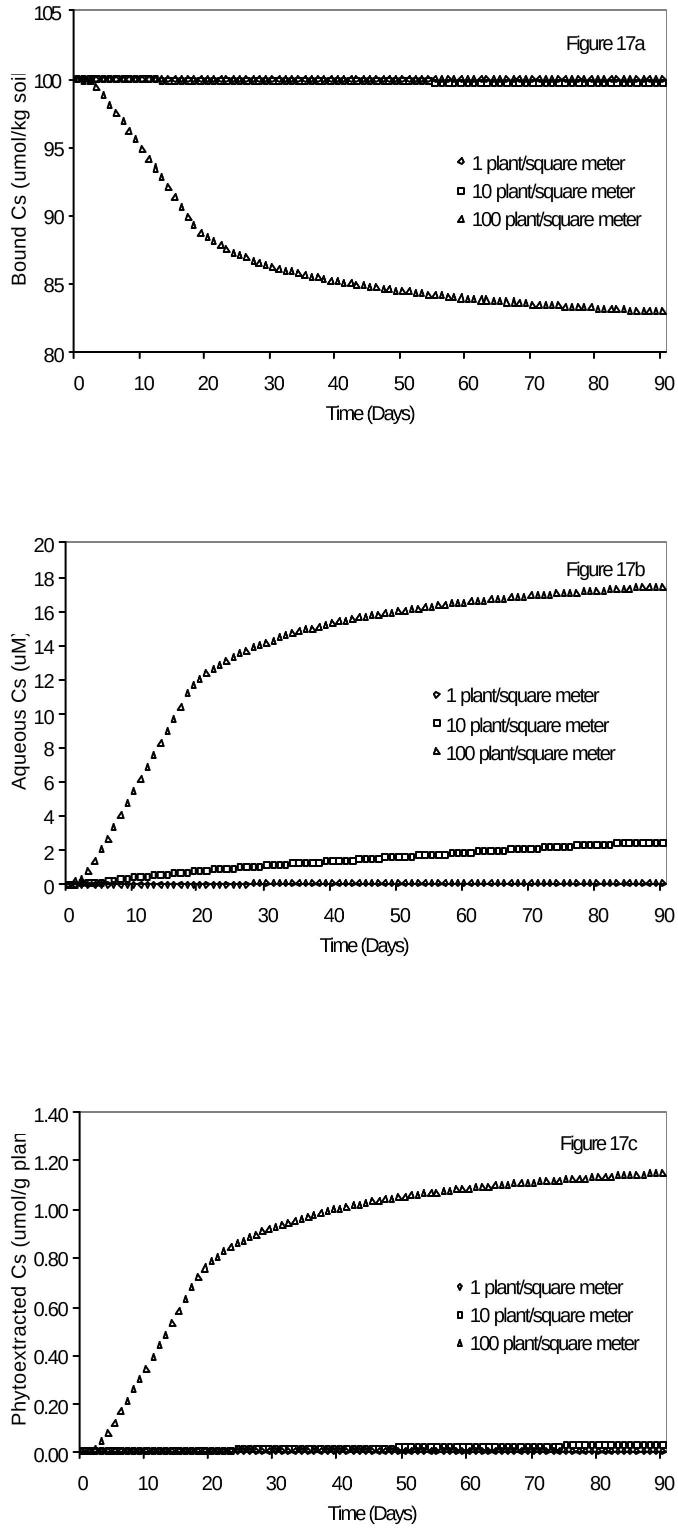

Figure 17. Effect of aerial plant density on Cs partitioning

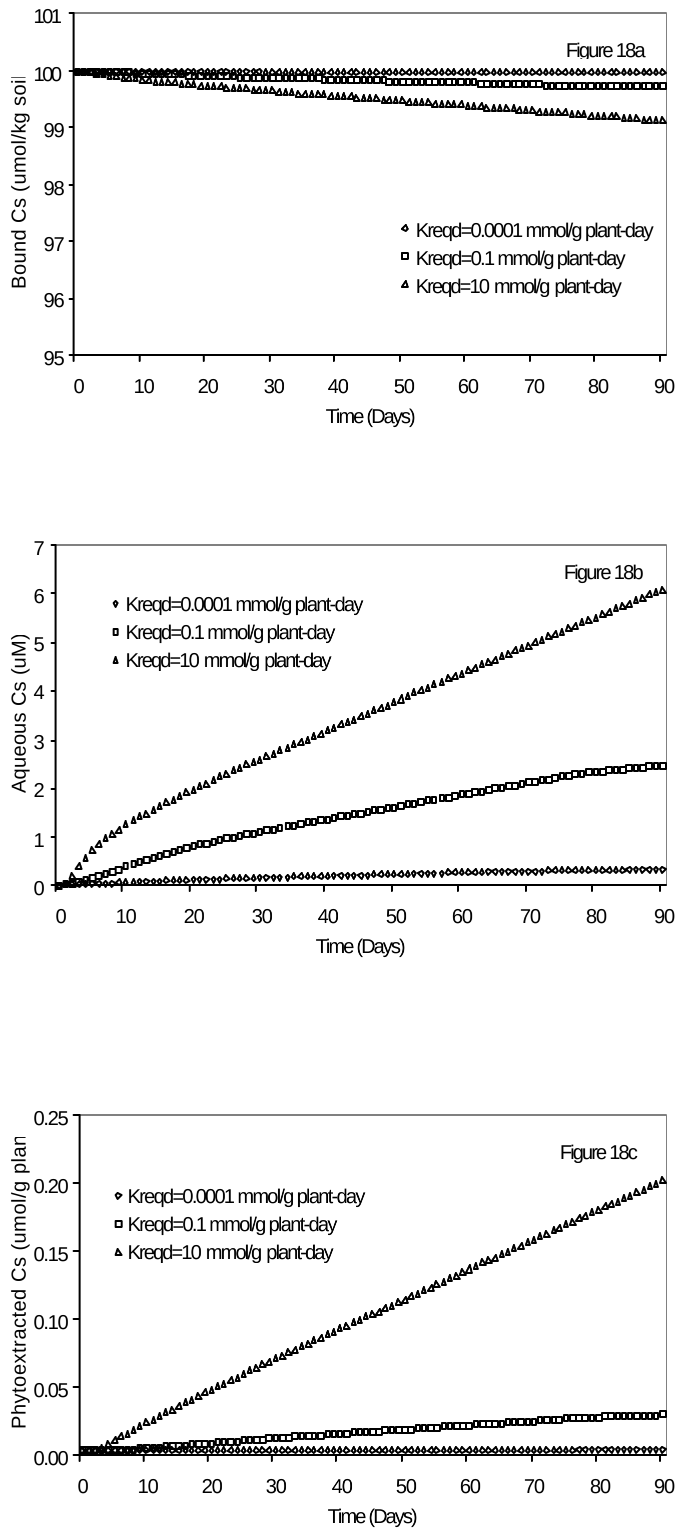

Figure 18. Effect of potassium required on Cs partitioning

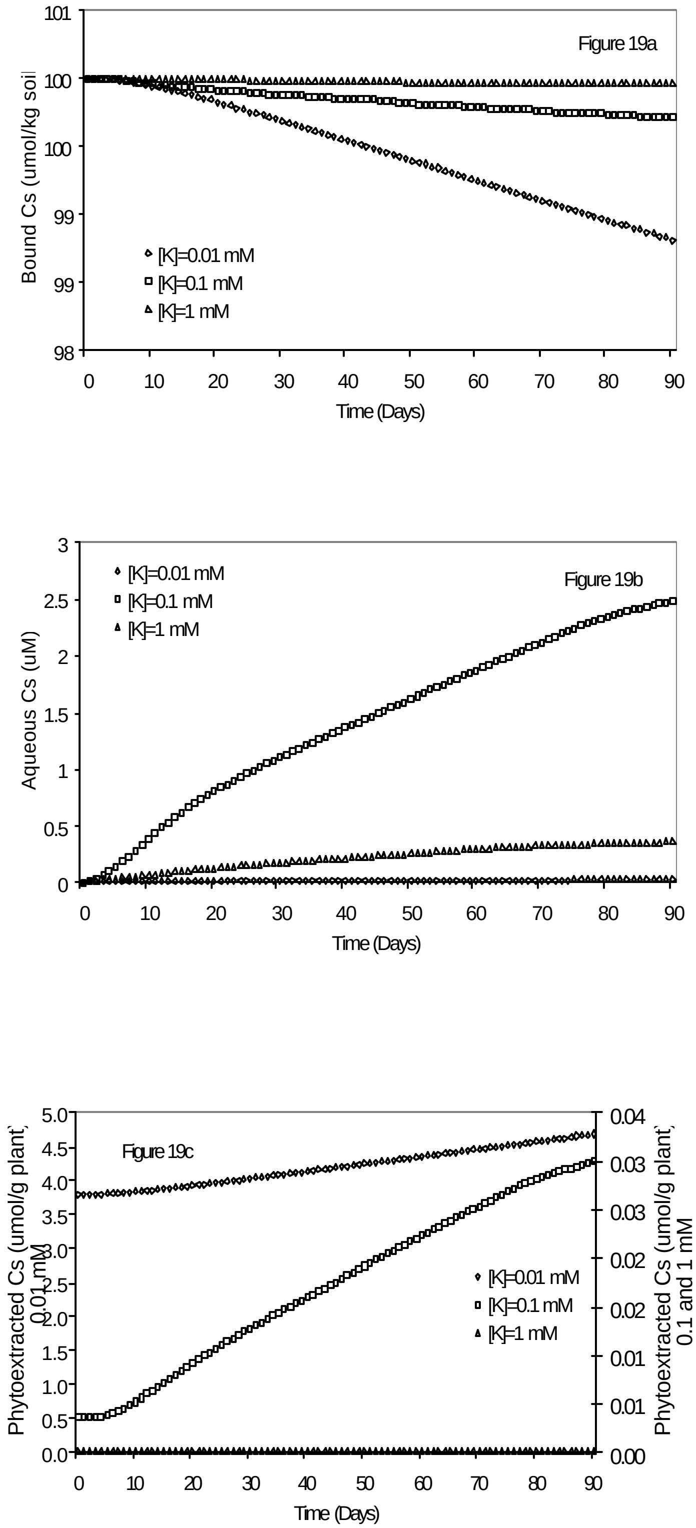

Figure 19. Effect of potassium concentration ([K]) on Cs partitioning

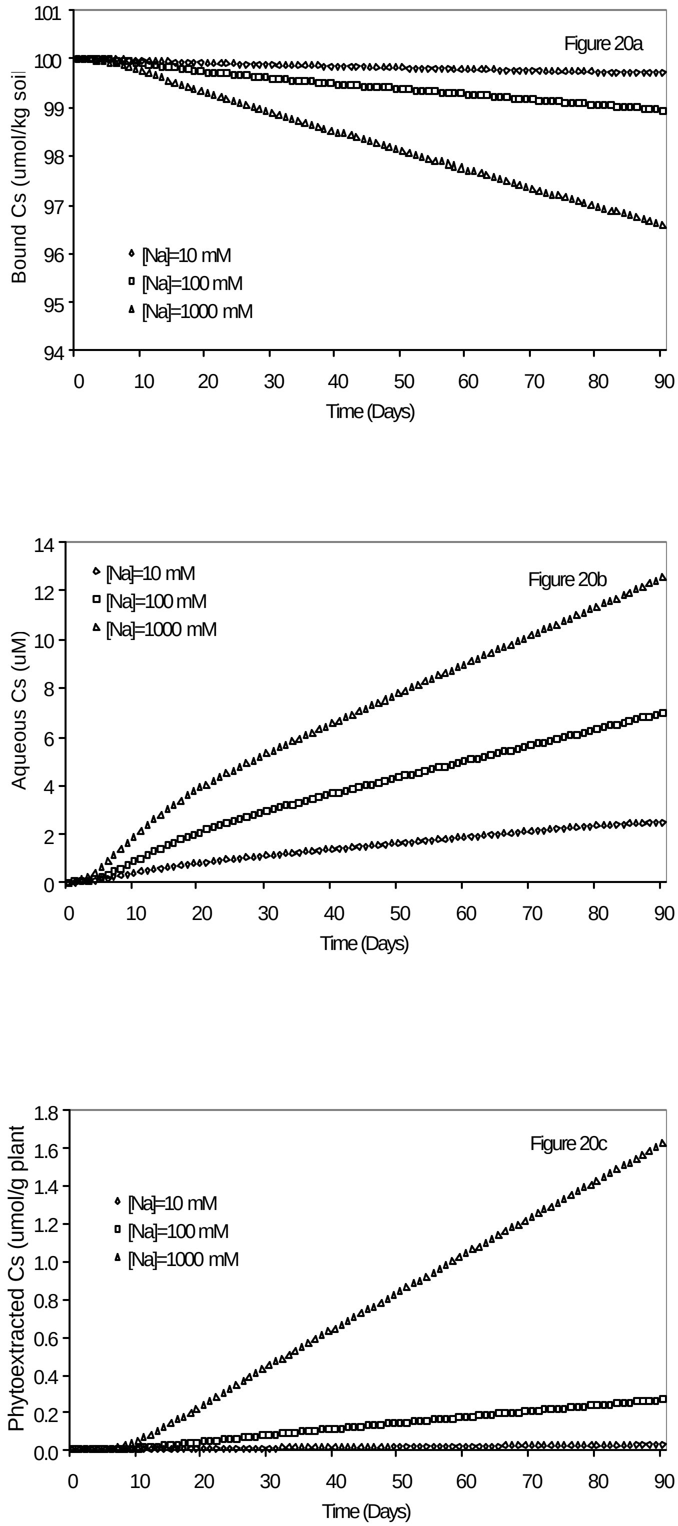

Figure 20. Effect of sodium concentration ([Na]) on Cs partitioning

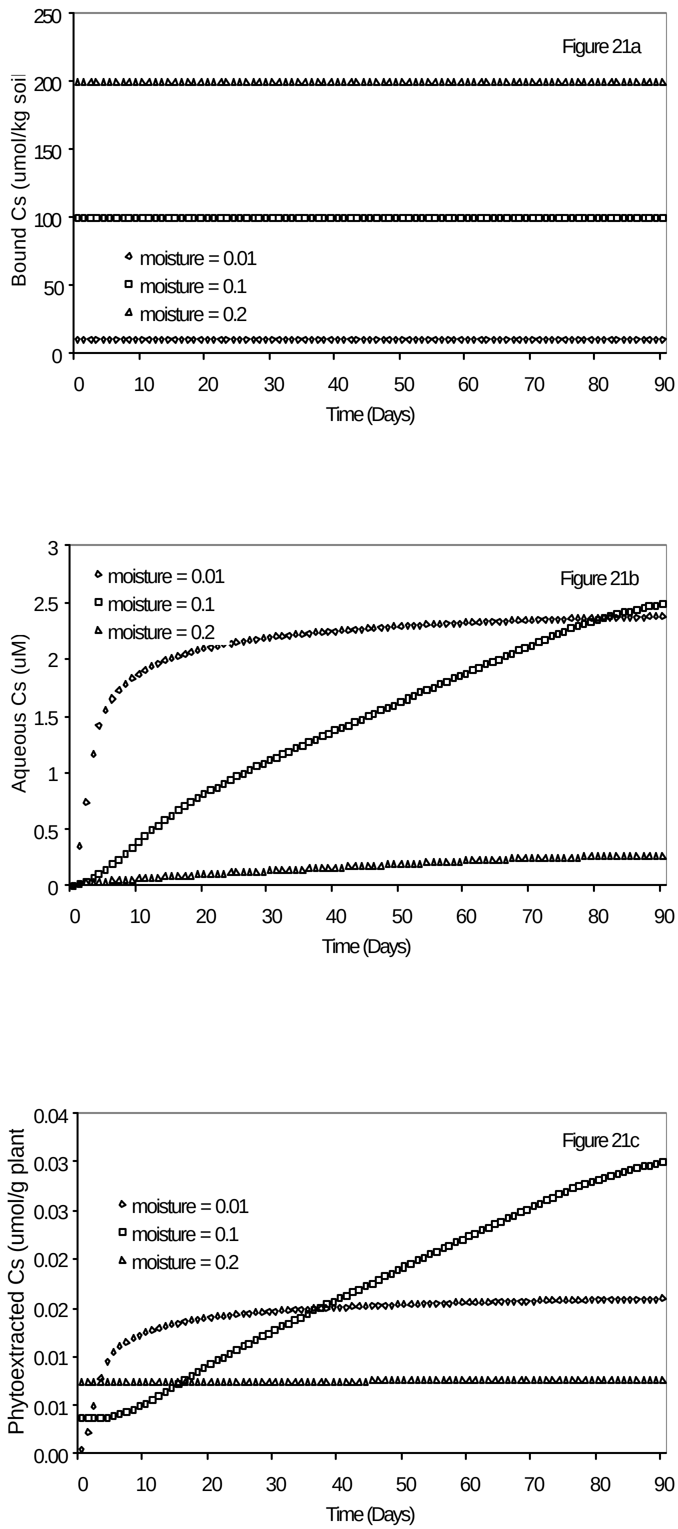

Figure 21. Effect of moisture on Cs partitioning

SUMMARY AND CONCLUSIONS

A System Dynamics model is presented as a framework for better understanding the complex interactions of processes that control Cs fate in the rhizosphere. The model is based on seven integrated sub-models for prediction of processes controlling cesium partitioning in the rhizosphere. Analyses tested the sensitivity of root exudates on Cs partitioning. Analyses also tested the sensitivity of root density, aerial plant density, potassium requirement and concentration, sodium concentration, and moisture content on the fate of root exudates and Cs. The overall affect of varying these factors on Cs partitioning is complex due to the many relationships involved.

Results of these sensitivity analyses may be used to optimize the remedial performance of the rhizosphere. Increasing root density and aerial plant density have similar effects on the system, i.e., affects partitioning by increasing [E] and $Flow_{phy}$. However, it is more practical to increase the amount of plants per area by planting more seeds, than it is to force each plant to grow more. Decreasing $[K^+]$, perhaps by eliminating fertilization, may induce stress, resulting in greater exudate release and greater phytoextraction. Increasing $[Na^+]$, perhaps by adding an innocuous sodium solution, decreases K_{ND}. However, with all of these approaches, caution must be heeded prior to field implementation. The entire model must be calibrated, followed by performing sensitivity analyses running each of the sub-models. Proceeding without this assessment may overlook complex interactions not seen by holding certain sub-models constant.

Currently, the model focuses on the role of root exudates on Cs solubilization, calibrating with data from literature where laboratory or field data are not available. To improve upon model robustness, additional experimental data should be collected and incorporated into the development of functional relationships and their parametric values. Furthermore, the level of sophistication of the other sub-models needs to be increased. With that, sensitivity analyses should evaluate the effects on parameters within the other sub-models and their consequent effects on Cs partitioning, just as has been presented in this dissertation for the root exudates. Finally, controlled field studies should be conducted to provide validation data.

Modeling the interacting processes affecting cesium partitioning in the rhizosphere will help to generate hypotheses concerning the behavior of cesium in actual complex field soils. Ultimately, the model will be a tool to effectively manage radiocesium contamination in vegetated, shallow soil systems. Future inclusion of other processes in the model will expand its utility and make the model applicable for other metals.

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