A mathematical model to assist phytoremediation management and evaluation

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Contents

Abstract

Phytoremediation is the use of plants and their associated microbes for environmental cleanup. The use of phytoremediation for soil cleanup faces a number of challenges of which leaching of soil contaminants below the rooting zone poses a significant environmental threat. Partitioning of contaminants between plant uptake and leaching is the focus of this Masters Project (MP). An improved mathematical model to represent phytoremediation processes are developed that couple the hydrological balance and soil contaminant balance for a dynamic vegetation system (i.e. rooting zone depth and leaf area are changing in time during the remediation period). Two different measures of phytoremediation efficiency are then assessed with different water supply amount & frequency, soil & plant properties and climatic conditions. It is found that water supply pattern is a first-order factor controlling the efficiency of phytoremediation when viewed from the perspective of maximizing plant-water uptake of contaminants. Climate change could also exert significant influence by affecting growth patterns of the plant. Additionally, a geospatial analysis tool is also created with the model to locate areas where phytoremediation may be an effective management option, when the climatic and soil datasets are available. With this combined geospatial tool and the newly proposed model, phytoremediation managers can evaluate the potential phytoremediation efficiency according to their specific situation.

1 Introduction

Phytoremediation is the use of plants and their associated microbes for environmental cleanup [19, 21]. It can be employed for degrading and sequestering both organic and inorganic pollutants in soil, water and air. Key mechanisms of phytoremediation may include [21]

- Phytostabilization: the use of plants to reduce the bioavailability of pollutants in the environment;
- Rhizofiltration: the use of plant roots to absorb and adsorb pollutants, mainly metals, from water and aqueous waste streams;
- Phytoextraction: the use of pollutant-accumulating plants to remove metals or organics from soil by concentrating them in harvestable parts;
- Phytodegradation: the use of plants and associated microorganisms to degrade organic pollutants;
- Phytovolatilization: the use of plants to volatilize pollutants.

These processes can be affected by plant species, soil properties, chemical properties of pollutants, climatic conditions, etc... Phytoremediation is a solar driven and environmentally friendly technique because it decontaminates without disturbing the physical, chemical and ecological characteristics of soils. Due to its cost-effectiveness and eco-friendliness compared to other solutions (e.g., pump-and-treat, dig-and-dump) phytoremediation has gained increasing popularity in many countries experiencing build-up of toxic pollutants (metals and organic contaminants in soil, surface water and ground water). Covering all aspects of phytoremediation design and best management practices (BMPs) is well beyond the scope of a single Masters Project (MP). This MP will primarily focus on **phytoextraction** and **rhizofiltration** though the issues considered here have direct bearing on all forms of phytoremediation.

The efficiency of phytoremediation is commonly evaluated in several ways and differing time scales. In several cases, the percent of contaminant removed over a certain period of time can be used. Another is the ability of the plant to translocate contaminants from roots to shoots. During phytoextraction or rhizofiltration of polluted soils, leaching of pollutants below the rooting-zone can lead to contamination of aquifers and surface water bodies that then leads to a significant environmental hazard. Hence, percent reduction of soil contaminants alone is not satisfactory as it cannot distinguish between the decline in soil contaminant concentration due to leaching and uptake by plants. Hence, quantification of the partitioning of soil contaminants between **leaching** and **plant uptake** is a necessary though not a sufficient step to evaluate phytoremediation efficiency - at least from a hydrological perspective.

A previous study [11] proposed a stochastic lumped model to evaluate the effect of rainfall patterns on phytoremediation efficiency, which is the first and only study to model such complex partitioning. The mathematical model of phytoremediation in this MP builds on this framework [11] but with a number of novel additions dealing with dynamic vegetation, the influence of toxicity on plant growth, and coupling the carbon and water economies of plants as needed to accommodate environmental drivers. The objective is to improve the quantification of the leaching-uptake partitioning and evaluate the suitability of phytoremediation for a broad spectrum of climatic conditions, soil and plant types and contaminant species. These additions will allow environmental managers and planners to assess whether phytoremediation is a viable alternative to conventional treatment and further consider management issues during the remediation (e.g. whether to irrigate the plant to maintain deterministic water supply).

2 Methods

2.1 The phytoremediation model

A lumped model is developed to represent the ecohydrological processes during phytoremediation. It includes three coupled components: a water balance describing soil moisture, soil contaminant concentration and plant biomass.

For simplification purposes, several assumptions are made:

- The water and contaminant mass balances within the rooting zone are horizontally-averaged and depth-integrated. Hence, detailed variation along the rooting depth are not explicitly treated. Water out of the rooting zone is assumed to be 'gravity-driven' dictated by the layer-averaged soil moisture in the rooting zone.

- The diurnal and seasonal fluctuation of environmental variables are not explicitly considered though the model can be revised to accommodate them.

- The contaminant accumulated in the plant is evenly distributed in roots and shoots. It is toxic to the plant by hindering transpiration.
- The above- and below- ground biomass of the plant follow an isometric scaling relation.
- Leaf area index (LAI) and mean rooting zone depth (Z_r) are proportional to the biomass of plant shoots and roots. Respiration rate of the plant is proportional to the total biomass. The assimilated carbon is distributed to roots and shoots with a constant ratio to form dry tissues.

The theoretical and empirical mechanisms of the model are described below. Definitions and symbols of different parameters of the model considered in this preliminary investigation are listed in Table 1. The model is available in MATLAB.

2.1.1 Hydrologic balance

The soil water hydrologic balance is [11]

$$nZ_r\frac{ds}{dt} = R - ET - LQ, \tag{1}$$

where n is the porosity of the soil; s is the degree of saturation measuring how much of the pore space is filled with water (between 0 and 1); Z_r is the mean rooting depth; R is the throughfall (or rainfall-interception); ET is the evapotranspiration from the soil-plant system; LQ are leakage or drainage fluxes from the rooting zone. Ponding and subsequent overland flow is ignored and it is assumed that the infiltration capacity of the soil exceeds rainfall throughout. In water limited cases, ET can be modelled with

$$ET = Tr + Ev \tag{2}$$

$$Tr = ET_{max} \cdot f(LAI)f(s) - tox \cdot UP_t \tag{3}$$

$$Ev = ET_{max} \cdot e^{-0.4LAI}\theta_R \tag{4}$$

$$\theta_R = \frac{s - s_w}{s_1 - s_w}, \tag{5}$$

where Tr is the plant transpiration; Ev is the evaporation from the soil surface; LAI is the leaf area index; tox is a factor that reduces transpiration based on contaminant uptake, indicating how strong the hindering effect of the total accumulated contaminant (UP_t) is on plant transpiration; θ_R is the relative soil moisture; s_w is the degree of saturation at the wilting point of the plant; s_1 is the degree of saturation at field capacity. Transpiration increases with LAI linearly and with s logistically, while evaporation is proportional to θ_R and decreases as LAI increases [17].

The LQ can be modelled as

$$LQ = K_{sat}\left(\theta_R\right)^{2b+3}, \tag{6}$$

where K_{sat} is the saturated hydraulic conductivity of the soil and b is a coefficient linked to the curvature of the soil water characteristic curve. Both variables depend on soil texture, and hence soil type [2].

2.1.2 Contaminant balance

The soil contaminant mass balance is given by [11]

$$Z_r \frac{dx}{dt} = -UP - LE, \tag{7}$$

where x is the total contaminant concentration, UP is plant uptake of contaminants, and LE is leakage of contaminants from the rooting zone.

The fluxes UP and LE can be modelled with [11]

$$UP = \kappa ET x_s \tag{8}$$

$$LE = x_s LQ \tag{9}$$

$$x_s = \frac{x}{ns + \rho_b K_d}, \tag{10}$$

where x_s is the contaminant concentration in the soil solution only; ρ_b is the bulk soil density; K_d is related to the adsorption isotherm of the contaminant under consideration; κ is known as the transpiration stream concentration factor [1] that varies with both the plant type and the contaminant.

2.1.3 Vegetation dynamics

The effects of dynamic vegetation lead to variable LAI and mean rooting depth, which depend on carbon assimilation by the plant. The rates describing carbon input, losses, and allocation are

$$A_n = Tr \cdot WUE \tag{11}$$

$$Re = (M_{sh} + M_{rt}) \cdot R_f \tag{12}$$

$$\frac{dM_{sh}}{dt} = \frac{f_{sh}(A_n - Re)}{C_C} \tag{13}$$

$$\frac{dM_{rt}}{dt} = \frac{f_{rt}(A_n - Re)}{C_C}, \tag{14}$$

where A_n and Re refer to net carbon assimilation and the plant's respiration respectively; WUE is the leaf-level water use efficiency, which depends on the stomatal resistance to carbon dioxide and water vapor [12], and is determined by atmospheric carbon dioxide concentration (C_a) and vapor pressure deficit (VPD) (i.e. $WUE \propto \frac{C_a}{VPD}$) described elsewhere [5, 6, 8]; R_f is a factor for converting mass to respiration rate; M_{sh} and M_{rt} are the dry tissue biomass of the plant's shoots and roots; f_{sh} and f_{rt} are the empirical proportion of assimilated carbon allocated to above- and below- ground biomass of the plant, assigned 0.75 and 0.25 respectively [15]; C_C is the concentration of carbon in dry matter, assigned a numerical value of 0.5 [20]. LAI and Z_r are proportion to M_{sh} and M_{rt} empirically [10, 18].

2.1.4 Contaminant fate and phytoremediation efficiency

Two measures of phytoremediation efficiency are adopted and compared. The concentration-based efficiency η_c that can be defined as the total decline in contaminant concentration (x) in the soil during the entire phytoremediation period (T) and is given by [4]

$$\eta_c = 1 - \frac{x(T)}{x(0)}, \tag{15}$$

where $x(0) = x_o$ is the concentration at time $t = 0$. The flux-based efficiency η_f can be defined as the proportion of plant uptake (UP) to total removal by moving water (i.e. plant uptake + leaching (LE)) and is given by [11]

$$\eta_f = \frac{\int_0^T UP(t)dt}{\int_0^T \left[LE(t) + UP(t)\right] dt}. \tag{16}$$

The η_c may be viewed as a traditional index to assess phytoremediation effectiveness. The more reduction in contaminant concentration occurs after a period T, $x(T)/x_0$ becomes small and η_c is closer to unity (i.e. high efficiency). The closer η_f is to unity, the more efficient is the plant uptake in the phytoremediation processes. Again, η_c does not distinguish between leaching and uptake, whereas η_f is primarily based on this distinction.

2.1.5 Summary

The newly developed model is illustrated in Figure 1, where the blue, red and green colors represent the hydrologic, contaminant and carbon/biomass balances, respectively. The toxic effect of the bio-accumulated contaminants in the plant tissues, which may hinder transpiration and consequently plant growth, is indicated with the red arrows. White components are external factors of the model whose influences on the model efficiencies are evaluated.

Table 1: Definition of variables in the phytoremediation model

Symbol	Definition	Units
b	empirical coefficient relating hydraulic conductivity and soil moisture	-
f_{sh}	portion of carbon allocated to above-ground biomass	-
f_{rt}	portion of carbon allocated to above-ground biomass	-
n	soil porosity	-
s	degree of saturation	-
s_w	degree of saturation at wilting point	-
s_1	degree of saturation threshold for initiating deep percolation	-
tox	parameter indicating toxicity effects on plants	-
x	total contaminant concentration	$g\ mm^{-3}$
x_s	contaminant concentration in soil solution	$g\ mm^{-3}$
A_n	net carbon assimilation	$kgC\ m^2\ d^{-1}$
C_C	Fraction of carbon in dry biomass	-
ET	evapotranspiration	$mm\ d^{-1}$
ET_{max}	maximum evapotranspiration	$mm\ d^{-1}$
LE	leaching losses	$g\ mm^{-2}\ d^{-1}$
K_d	slope of the linear adsorption isotherm, $x - x_s = K_d x_s$	$m^3\ g^{-1}$
K_{sat}	reference hydraulic conductivity close to saturation	$mm\ d^{-1}$
LAI	leaf area index	$m^2\ m^{-2}$
LQ	deep percolation	$mm\ d^{-1}$
UP	contaminant uptake by plants	$g\ mm^{-2}\ d^{-1}$
M_{sh}	above-ground biomass	$kg\ mm^{-2}$
M_{rt}	below-ground biomass	$kg\ mm^{-2}$
R	rainfall	$mm\ d^{-1}$
Re	respiration	$kgC\ m^2\ d^{-1}$
R_f	factor of respiration to total biomass	-
WUE	water use efficiency	-
Z_r	mean rooting depth	mm
κ	transpiration stream concentration factor (TSCF)	-
ρ_b	soil bulk density	$g\ m^{-3}$

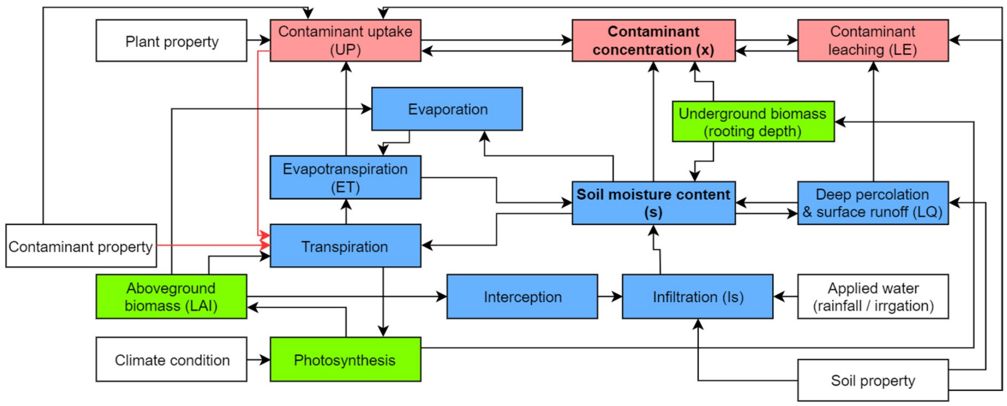


Figure 1: The phytoremediation model with a dynamic vegetation component and feedback between contaminant uptake and transpiration

Table 2: Parameter values assumed for the case study

Temperature	25°C
Atmospheric CO_2	400 ppm
Annual precipitation	800 mm
Precipitation return period	10 d
ET_{max}	4 mm/d
Initial s	0.7
Soil type	Sandy clay loam
TSCF	0.54
Model period	365 d

2.2 A phytoremediation case study

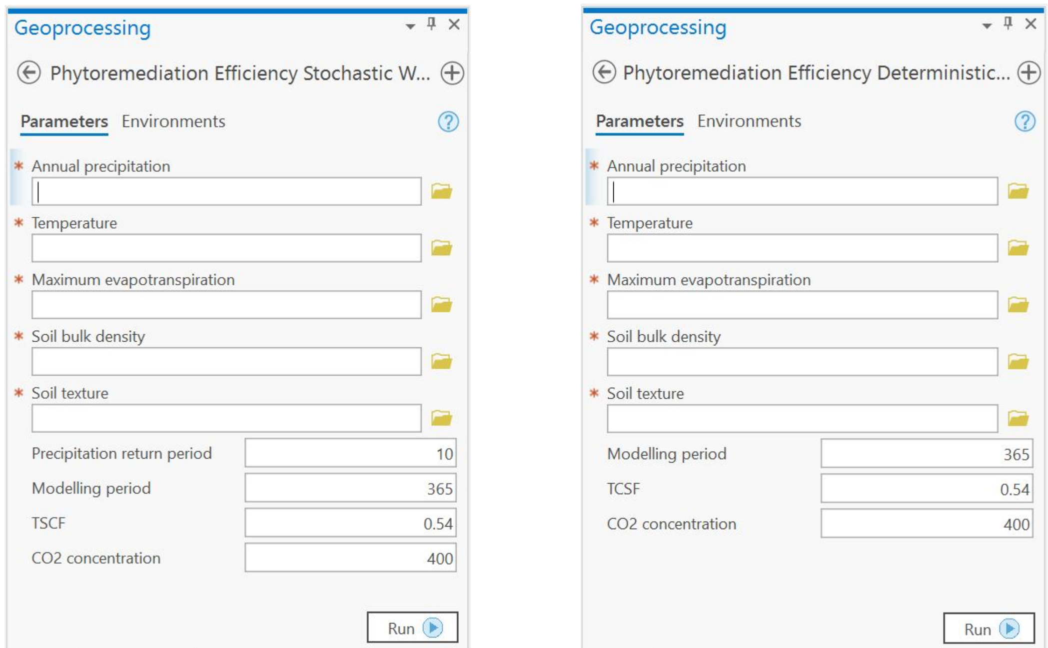
The analyses reported here are based on a case using barley (*Hordeum vulgare* L.) as a crop to clean a soil polluted by Aldicarb, a carbamate insecticide. The assumed values of the parameters are listed in Table 2. It should be noted that these parameters can be adjusted for different crops, contaminants and for different environments.

Sensitivity analyses are conducted on the environmental parameters including water supply pattern, climatic, edaphic and plant properties. Specifically, the water supply source is expanded to include deterministic or constant input of water so that anthropogenic management measures (e.g. irrigation) can be represented. This case also offers a base-line run to assess the role of rainfall stochasticity on the two efficiency measures. Total amount of water applied during a certain period and its frequency / return period are also considered in the stochastic rainfall model runs. The model is operated on a daily time scale with rainfall amounts and inter-pulse duration assumed to be derived from an exponential distribution with externally described means (annual mean and return period of storms). This assumption precludes storms with duration exceeding 1 day. It also assumes that storms are not correlated in time on daily and longer time scales. Some justification of these assumptions for North Carolina are featured elsewhere [7]. Seasonal variations in rainfall can be readily accommodated in this model but are momentarily ignored here.

2.3 A geospatial tool to evaluate phytoremediation suitability

With climatic and soil data maps available, a geospatial pattern of phytoremediation potential efficiency can be generated with ArcGIS. Here, the GIS tool is developed by applying the model within Python (Figure 2) so that phytoremediation managers can use it to determine where it is suitable to adopt phytoremediation to clean the soil (at least from an anticipated efficiency perspective).

North Carolina (NC) is used as an example region. The annual spatial



(a) For stochastic precipitation (b) For deterministic precipitation

Figure 2: GIS tools to generate map of phytoremediation efficiency

distribution of mean air temperature, cumulative annual rainfall [16], potential evapotranspiration [14] as well as soil texture maps [3] are assembled into a GIS and interfaced with the model. A map showing the spatial patterns of the two phytoremediation efficiencies is then determined across the entire state. To be clear, this map must be viewed as a 'potential efficiency' because numerous other factors that can impact placement decisions of phytoremediation sites are excluded.

3 Results and discussion

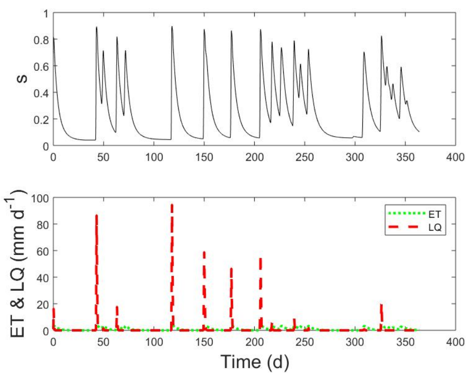
3.1 A case of simulated phytoremediation

Figure 3 show the modelled variables impacting the phytoremediation process under a stochastic rainfall water supply. Figure 3a presents the key state and flux variables for the hydrologic, carbon/biomass and contaminant balances. During the phytoremediation process, the soil degree of saturation (s) fluctuates with rainfall events. The hydrologic fluxes, evapotranspiration (ET) and deep drainage (LQ) are also depicted. Deep drainage occurs when the incoming water leads to excess saturation above and beyond the field capacity. The plant leaf area index (LAI) and mean rooting depth (Z_r) are increasing over time (Figure 3c). The change in soil contaminant concentration and its key fluxes, plant uptake (UP) and leakage (LE) are shown in Figure 3b. UP and LE are elated with ET and LQ. The three budgets interact with each other and exert controls on plant growth. In the case featured here, the two efficiencies are η_c of 0.42 while η_f is 0.48.

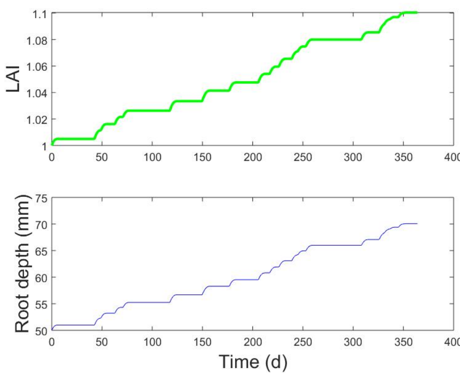
3.2 Model evaluation

It is challenging to test the model performance and verify its assumptions. There are hardly any published empirical studies that simultaneously report climatic variables, plant variables, hydrologic fluxes, and contaminant fluxes.

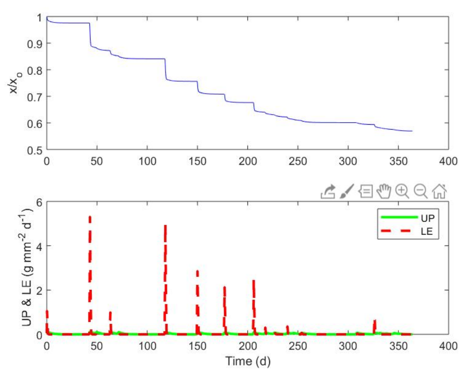
While less ideal, a designed pot experiment conducted by Luo et al. [9] can be used to assess the model performance qualitatively. In this experiment, multiple assisting techniques are applied in a heavy metal decontamination with *Eucalyptus globulese*. The experiment applies water at a large



(a) Hydrology dynamics



(b) Vegetation dynamics



(c) Contaminant dynamics

Figure 3: Modelled state variables and fluxes impacting the phytoremediation processes for a stochastic water supply. Dependent variables are the value of key states and fluxes; dependent variable is time (in days).

rate of 25 mm per day for 14 days. The quantity of initial soil contaminant, bio-accumulated and leached contaminant were measured, which is one of the main reasons this experiment is used to assess model performance. Calculated from the provided data, the η_c for various contaminants Cd, Pb and Cu are in the range of 0.03 to 0.13; the η_f for Cd, Pb and Cu are in the range of 0.26 to 0.59.

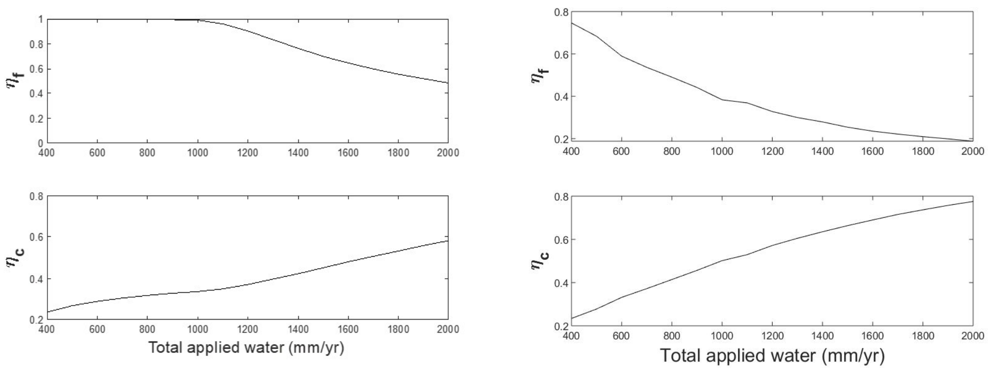
If we run the model with the Barley - Aldicarb case with such precipitation pattern, it yields an η_f of 0.1 and η_c of 0.3. The inverse relation between η_c and η_f reported is also reasonably captured. Comparing the model outcomes with these measurements is akin to comparing 'apples' and 'oranges' as the climate, plant and soil properties are not the same (much information was not disclosed in the experiment). However, this comparison is suggestive that the model results are not deviating appreciably from expectations in terms of order of magnitude for the two efficiencies.

3.3 Sensitivity analysis of phytoremediation efficiency to environmental conditions

3.3.1 Precipitation statistics

Constant precipitation Figure 4a shows that as the total amount of water changes, η_f for the aforementioned case decreases while η_c increases. This outcome is not surprising since there is more leaching as the entering water exceeds the holding capacity of the soil. The increased leaching makes up most of the increase in total removal, or η_c.

Noteworthily, η_f is nearly 1 when the quantity of total applied water is



(a) Constant water supply

(b) Stochastic water supply

Figure 4: Change in phytoremediation efficiency with total amount water applied

below an annual critical value, which is around 1000 mm/yr in this case (i.e. based on the soil-plant system). This critical value actually represents how much water can the bulk of soil holds so it is mainly determined by the soil category. When the total applied water is less than the critical value, η_f is high and insensitive to other environmental variables.

Stochastic precipitation When the water supply is stochastic, the trend of the efficiencies are similar to the constant scenario, but η_f is generally lower and η_c higher (Figure 4b), because the entering amount of water of a single precipitation event can be much higher, which could cause both drainage and subsequent leaching. The more unevenly the water is distributed temporally (i.e. the same amount of water is applied with low frequency and long return period), the further would η_f drop (Figure 5) consistent with logical expectations. These findings underscore the significance of the soil-plant system and the precipitation regime when considering phytoremediation options.

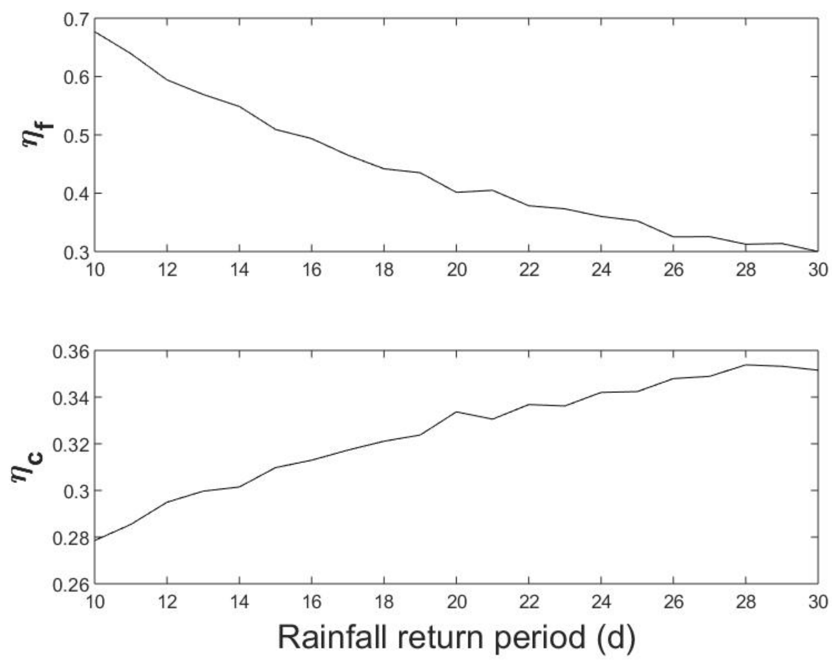


Figure 5: Change in phytoremediation efficiency with return period of stochastic water supply

3.3.2 Soil type

In the model, soil texture determines the porosity, hydraulic conductivity and degree of saturation at wilting point. Hence, it controls infiltration and deep drainage of water, and thereby the leaching of contaminant. The results from the model reveal that as the soil type changes from clay to sand, η_f drops while η_c rises (Figure 6) when all other factors are maintained the same. Moreover, the rate of change is large for coarse soils. Therefore, a soil coarser than sandy loam is much less suitable for phytoremediation as soil water drains out quickly and η_f abates drastically.

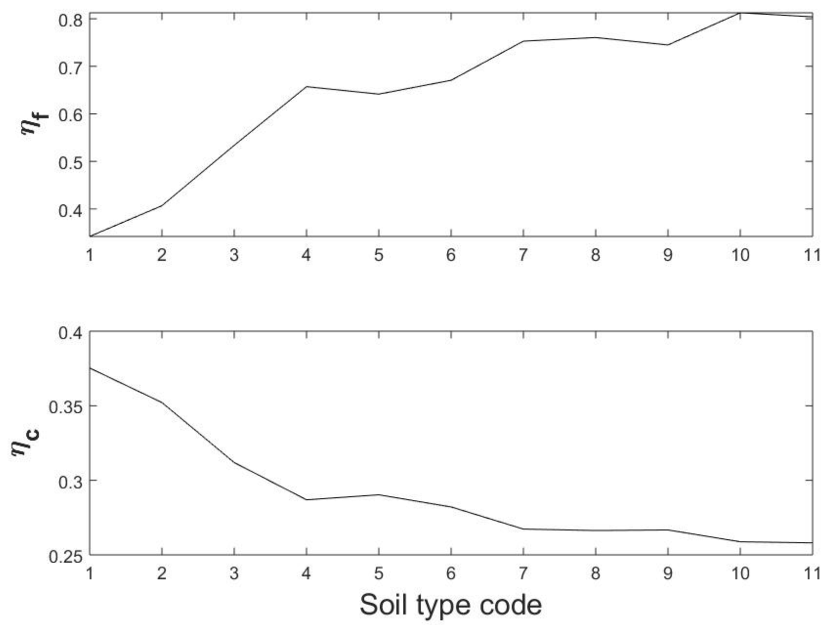


Figure 6: Change in phytoremediation efficiency with soil type under stochastic water supply. Soil type 1 to 11 represent progressively changes from sand to clay. See Appendix A for the representation of each code.

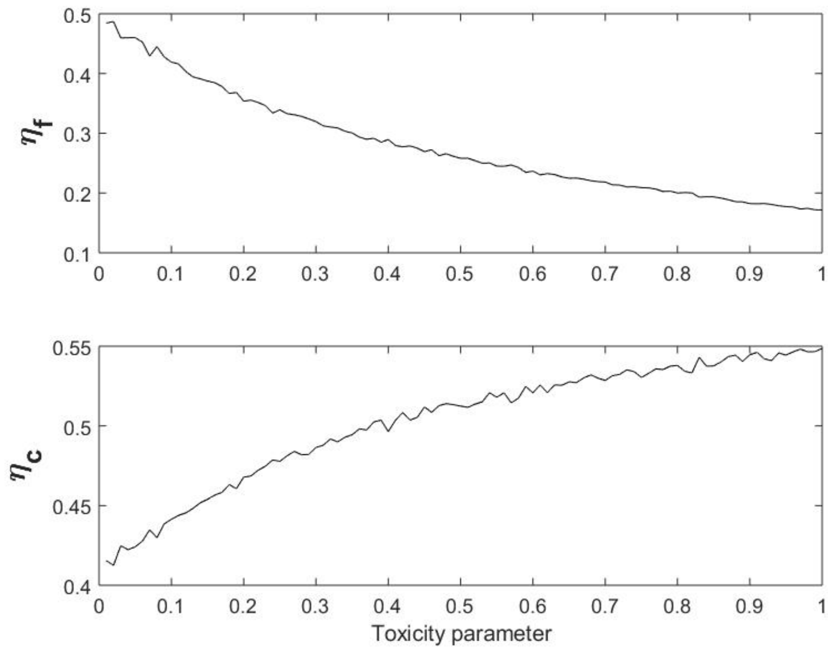


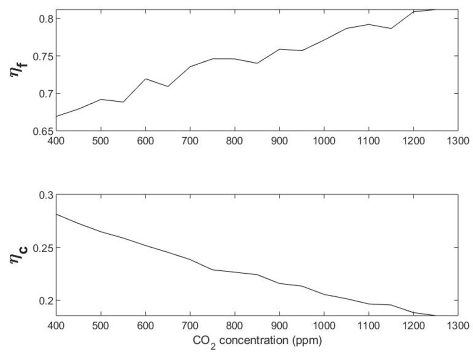
Figure 7: Change in phytoremediation efficiency with toxicity parameter (tox) under stochastic water supply. The larger tox is, the more toxicant the contaminant is, or the less tolerant the plant is.

3.3.3 Contaminant toxicity / Plant tolerance

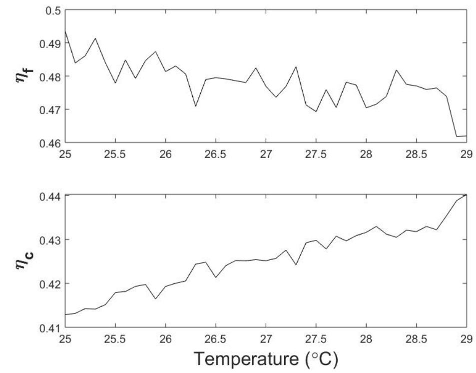
The plant growth would be slowed by accretion of absorbed contaminant in the plant tissues. If the the contaminant species is more toxic to the plant, or the plant is less tolerant to the toxicity, η_f would drop and η_c enlarges due to more leaching (Figure 7).

3.3.4 Climate

Within the dynamic vegetation model, climate factors are introduced as external variables that influence the plant growth so that it is possible to eval-



(a)



(b)

Figure 8: The effect of climatic variables such as atmospheric carbon dioxide C_a (left) and air temperature (right) on phytoremediation efficiencies under a stochastic water supply. The maximum temperature and C_a shown here follows IPCC's high green house gas emission scenario - Representative Concentration Pathway (RCP) 8.5 [13].

uate the effect of climate change on phytoremediation efficiency. For greenhouse phytoremediation, managers are able to adjust some factors to attain maximum efficiency.

Since the interaction between climatic variables is another complex issue, this MP only assess the sensitivity of phytoremediation efficiencies to each of them in isolation. Figure 8a shows that an elevated atmospheric carbon dioxide concentration (C_a) leads to higher η_f and lower η_c. An explanation is that elevated C_a increases WUE and facilitates the plant growth. As the mean rooting depth (Z_r) grows, the soil is able to hold more water. The effect of higher air temperature, however, is to decrease η_f and raise η_c (Figure 8b), for high temperature generates high vapor pressure deficit and thereby low WUE. This effect is more manifest for constant water supply condition (see Appendix B).

3.3.5 Dynamic vs Static vegetation

A comparison between the new dynamic vegetation model and the static vegetation model suggests that dynamic vegetation generates higher η_f and lower η_c, but the discrepancy is not huge. This result suggests that the simpler constant vegetation parameter can be used in the geospatial analysis to generate phytoremediation efficiency maps with reduced computational complexity.

3.4 Geospatial analysis of phytoremediation efficiency

The phytoremediation efficiency maps for North Carolina using a Barley crop and Aldicarb contaminant is shown in Figure 9. The maps use soil texture, annual rainfall, rainfall return period, air temperature, vapor pressure deficit, and maximum evapotranspiration as model input. Both efficiencies vary spatially consistent with the large soil type variation and climatic conditions. Broadly, where η_f is higher, η_c is lower. The Coastal Plain has relatively low η_f and high η_c, while the Piedmont region has relatively high η_f and low η_c. In the Mountains, the pattern is correlated with the rainfall, indicating that rainfall is the most influential factor in the region. For some noticeable patches in the Coastal Plain, however, soil type is the dominantly deterministic factor.

4 Conclusions and Suggestions

Based on the model and results featured here, the following recommendations are offered to phytoremediation managers.

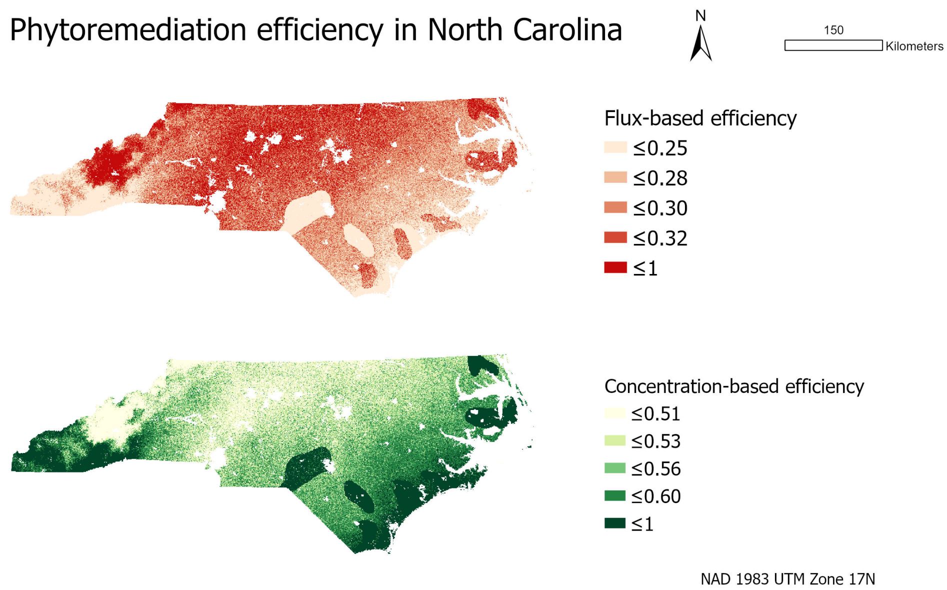


Figure 9: The spatial pattern of phytoremediation efficiencies in NC

First, the pattern of water supply is a leading order consideration for phytoremediation and impacts the efficiency in a nonlinear manner. Current trends in phytoremediation research focus on cutting-edge techniques to improve efficiency such as gene modification, chelator application and electric field assistance. However, a simpler hydrologic optimum can facilitate phytoremediation effectively. Typically, contaminant uptake is maximized at a critical uniform water supply as described in 3.3.1. Therefore, managers may adopt either measures to buffer precipitation or supplementary irrigation to control the water applied to the plant.

Second, as external environmental conditions change, the two types of efficiency are inversely related. That is, there is a trade-off between concentration-based and uptake-based efficiencies. This modelled relation is in accordance with the results disclosed by pot-studies [9]. Managers need to evaluate which efficiency is to be maximized, and this can be problem specific. If the goal is to reduce root-zone concentration without considerations to the role of leaching, then the conventional concentration-based efficiency may be preferred. If the goal is to maximize plant uptake and minimize leaching, then the flux-based efficiency is preferred. Naturally, the fragility of the local groundwater system to pollution cannot be ignored in this assessment. If groundwater levels are available, they can also be accommodated in the geospatial analysis proposed here.

Third, the proposed phytoremediation model can be interfaced with a geospatial analysis tool to decide optimal phytoremediation location as long as necessary environmental data and soil maps are available. The tool can be handy to phytoremediation managers and the code will be made public via GitHub.

5 Prospects

The model proposed here is the first phytoremediation model to accommodate dynamic vegetation and stochastic precipitation. There are several aspects that warrant future studies.

When exploring the deterministic water supply scenarios, we found that with constant water input, the dynamical system will approach a steady state (see Appendix B) provided the modeling period is sufficiently long. This means that it is possible to explore this key equilibrium state in analyzing climatic forcing or model parameters (e.g. bifurcation type). Specifically, if it is assumed that the plant growth can be negative (declining biomass) with plentiful contaminant accumulated in its tissues, the plant would either reach its maximum biomass or die out (two-states in this system). The initial conditions, including the initial contaminant concentration in the soil, determine which equilibrium the system would approach. It is indicated that critical thresholds exist for a certain phytoremediation system that determine the fate of the system. This point is not covered in this MP, but should be considered as it can serve as important guidance for phytoremediation managers' decision-making.

The model and analysis can also be improved in several ways.

The current model is a lumped model, that the hydrology and contaminant balances are depth-integrated and horizontally averaged. While this approach is a logical starting point, a layer-resolving model can be developed so that detailed variation along the rooting depth are not averaged-out.

There are many simplifications for the processes and parameterization of variables, each of which can be expanded to provide more realistic simulation. For example, the relocation of contaminant inside the plant is not considered. Additionally, there is only one parameter indicating the toxicological effect on plant growth. This alone can be a complicated issue.

The synergetic impacts of environmental variables may be modeled to evaluate their joint effects more reasonably. For example, atmospheric carbon dioxide concentration, temperature and relative humidity can be coupled together with reliable modeling methods.

Acknowledgement

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Appendices

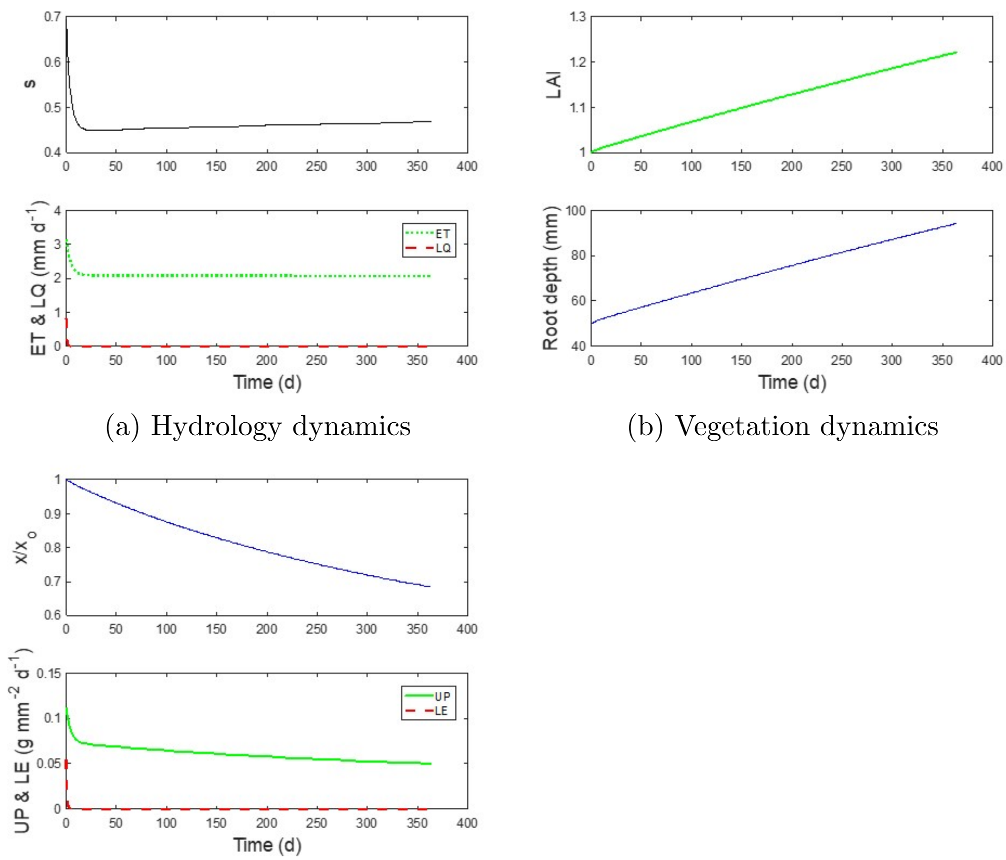
A. Soil code representations

Table 3: Soil code representations [2]

Soil code	Soil type
1	sand
2	loamy sand
3	sandy loam
4	silt loam
5	loam
6	sandy clay loam
7	silty clay loam
8	clay loam
9	sandy clay
10	silty clay
11	clay

B. Example dynamics and sensitivity analysis for constant water supply

To be concise, the main body of the MP report only presents the cases under stochastic water supply. Here the results for constant water supply are included.



(a) Hydrology dynamics

(b) Vegetation dynamics

(c) Contaminant dynamics

Figure 10: Modelled state variables and fluxes impacting the phytoremediation processes for a constant water supply. Y axes are the value of key state and flux variables; X axes are all time.

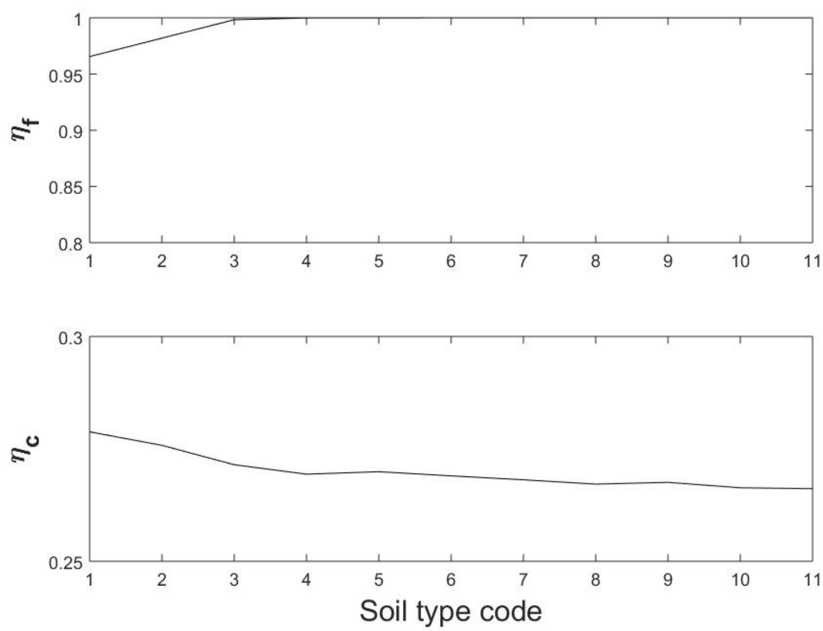


Figure 11: Change in phytoremediation efficiency with soil type under constant water supply. Soil type 1 to 11 represent sand to clay.

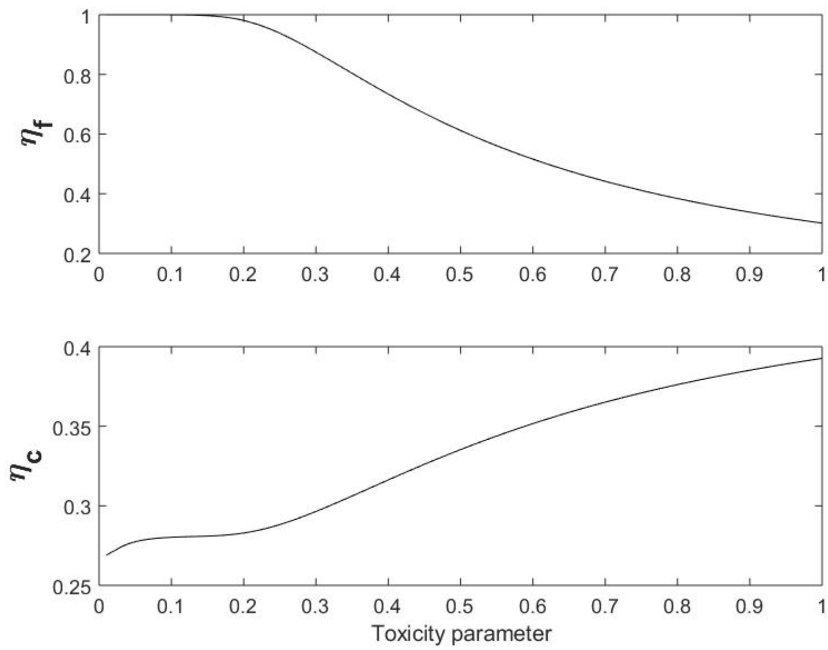
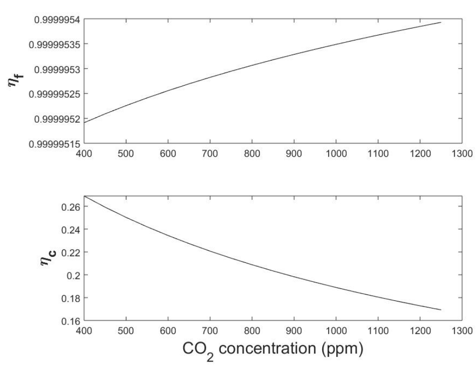
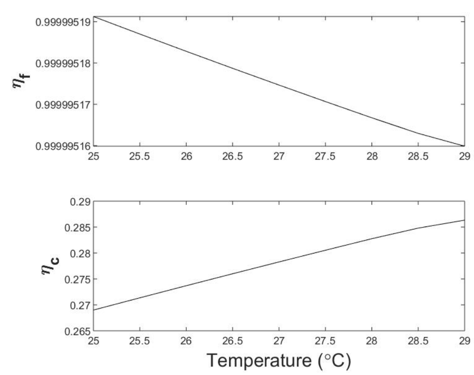


Figure 12: Change in phytoremediation efficiency with toxicity parameter (tox) under constant water supply. The larger tox is, the more toxicant the contaminant is, or the less tolerant the plant is.



(a) Change in phytoremediation efficiency with C_a



(b) Change in phytoremediation efficiency with temperature

Figure 13: The effect of climatic variables on phytoremediation efficiencies under stochastic water supply. Since the annual applied water (800 mm) is less than the critical value, η_f is close to 1 and not as sensitive to climate change as when the water supply is stochastic.