Nutrient Uptake Estimates for Woody Species as Described by the NST 3.0, SSAND, and PCATS Mechanistic Nutrient Uptake Models

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Abstract

With the advent of the personal computer, mechanistic nutrient uptake models have become widely used as research and teaching tools in plant and soil science. Three models NST 3.0, SSAND, and PCATS have evolved to represent the current state of the art. There are two major categories of mechanistic models, transient state models with numerical solutions and steady state models. NST 3.0 belongs to the former model type, while SSAND and PCATS belong to the latter. NST 3.0 has been used extensively in crop research but has not been used with woody species. Only a few studies using SSAND and PCATS are available. To better understand the similarities and differences of these three models, it would be useful to compare model predictions with experimental observations using multiple datasets from the literature to represent various situations for woody species. Therefore, the objectives of this study are to: (i) compare the predictions of uptake by the NST 3.0, SSAND, and PCATS models for a suite of nutrients against experimentally measured values, (ii) compare the behavior of the three models using a one dimensional sensitivity analysis; and (iii) compare and contrast the behavior of NST 3.0 and SSAND using a multiple dimensional sensitivity analysis approach. Predictions of nutrient uptake by the three models when run with a common data set were diverse, indicating a need for a reexamination of model structure. The failure of many of the predictions to match observations indicates the need for further studies which produce representative datasets so that the predictive accuracy of each model can be evaluated. Both types of sensitivity analyses suggest that the effect of soil moisture on simulation can be influential when nutrient concentration in the soil solution (C_{Li}) is low. One dimensional sensitivity analysis also revealed that I_{max} negatively influenced the uptake estimates from the SSAND and PCATS models. Further analysis indicates that this counter intuitive response of I_{max} is probably related to low soil nutrient supply. The predictions of SSAND under low-nutrient-supply scenarios are generally lower than those of NST 3.0. We suspect that both of these results are artifacts of the steady state models and further studies to improve them, such as incorporating important rhizospheric effects, are needed if they are to be used successfully for the longer growth periods and lower soil nutrient supply situations more typical of woody species.

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Chapter I. INTRODUCTION

Influenced by many chemical, physical, and physiological factors, plant nutrient uptake is a very complex process (Barber 1995). A mechanistic nutrient uptake model simulates this process using mechanistic or empirical equations based on basic mechanisms. Based on the seminal efforts by Nye and Marriot (1969) and Baldwin et al. (1973), and advanced by the subsequent work of Claassen and Barber (1976), Nye and Tinker (1977), Barber and Cushman (1981), Claassen et al. (1986), Smethurst and Comerford (1993), Yanai (1994), Smethurst et al. (2004), and Comerford et al. (2006), mechanistic models were developed for the personal computer that allows nutrient uptake by plant roots to be calculated. These models take into consideration the competition between roots within a specified time, as well as the size and growth of the roots, the kinetics of nutrient uptake, and the supply of nutrients from the soil to the root surface (Barber 1995). Research on several crop species has demonstrated that the predictions of these mechanistic models generally match the observed uptake under situations in which the soil and plant conditions are relatively constant (Barber 1995; Tinker and Nye 2000). Results with woody species have been more variable (Gillespie and Pope 1990; Van Rees et al. 1990; Smethurst and Comerford 1993).

Validated mechanistic models allow data interpolation and extrapolation (Claassen and Steingrobe 1999), and are able to provide predictions under various situations, which may avoid the need for costly field trials (Barber 1995; Tinker and Nye 2000). They can also be used to calculate values that are difficult to determine experimentally (Claassen and Steingrobe 1999) in addition to revealing the factors that have the greatest influence on the nutrient uptake processes (Barber 1995).

NST 1.0, SSAND, and PCATS are three mechanistic nutrient uptake models which were presented in 1986, 2000, and 2004, respectively (Li and Comerford 2000; Smethurst et al. 2004; Claassen et al. 1986). NST 3.0 is the improved version of NST 1.0, which was developed in 1990s and not published in a journal (Claassen, N. Personal communication. 2009, 31 July). NST models are based largely on the Barber-Cushman model (Claassen et al. 1986), and belong to transient state models using a numerical

solution. SSAND and PCATS are steady state models based on the key equations developed by Baldwin et al. (1973) and Nye and Tinker (1977), with the assumption that the "concentration profile around the root can be considered to be in a steady state" (Yanai 1994). Compared to SSAND, PCATS further simplifies calculation by running on a fixed daily time-step (Smethurst et al. 2004). Transient state models with a numerical solution are generally considered to be more accurate than steady state models (Smethurst and Comerford 1993; Yanai 1994). However, steady state models can be constructed to allow parameters to change during simulation and thus are able to respond to real-time changes in parameters as well as allowing for the feedback between soil and plant processes during simulation (Yanai 1994).

One way to evaluate the models is by comparing model predictions with measured values. A second way is to use sensitivity analysis. The traditional way to conduct a sensitivity analysis in the modeling context is to vary a single input parameter in a model while keeping the others constant (Silberbush and Barber 1983). By plotting the change ratio of the parameters compared to their original values on the horizontal axis, and that of the predicted uptake to the original prediction on the vertical axis, it is possible to evaluate the importance of each parameter by the slopes of the lines on the graph (Silberbush and Barber 1983). As Williams and Yanai (1996) have suggested, this method can be called a one dimensional sensitivity analysis. However, because the relative importance of parameters defined this way can depend strongly on the values of the other parameters, Williams and Yanai (1996) developed a multiple dimensional sensitivity analysis in order to study model behavior across a broad range of possible parameter values.

In their approach to multiple dimensional sensitivity analysis, Williams and Yanai (1996) utilized data taken from the literature for both crop and tree species. They identified four factors as the most influential parameters controlling uptake per unit length of root: (i) the average dissolved nutrient concentration (C_{av}), (ii) the maximal rate of nutrient uptake (I_{max}), (iii) the effective diffusion coefficient (D_e), and (iv) the root radius (r_0). However, as noted by Fitter (2002), differences between the roots of woody and herbaceous species can be important, especially in terms of root radius and

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suberization. Both of these differences could influence estimated nutrient uptake. Also, Williams and Yanai (1996) used a simplified model whose behavior may be different from the NST 3.0, SSAND, and PCats models. For example, the study by Van Rees et al. (1990) on slash pine (*Pinus elliottii* var. *elliottii*) and that of Kelly et al. (1992) on loblolly pine (*Pinus taeda*) indicate that the influence of root growth rate (k) is prominent in the sensitivity analysis by the NUTRIENT UPTAKE model by Oates and Barber (1987).

Most studies to date have focused on tests of individual models. The number of studies using SSAND and PCATS are limited. NST 3.0 has been widely used but only with crop species. Therefore, using a common data set to compare the predictions of nutrient uptake by NST 3.0, SSAND, and PCATS against observed values combined with the use of sensitivity analysis would help us better understand model behaviors under various situations and provide useful information for future model development.

Therefore, the objectives of this study are to: (i) compare the predictions of uptake by the NST 3.0, SSAND, and PCATS models for a suite of nutrients against experimentally measured values, (ii) compare the behavior of the three models using a one dimensional sensitivity analysis; and (iii) compare and contrast the behavior of NST 3.0 and SSAND using the multiple dimensional sensitivity analysis approach of Williams and Yanai (1996). Common data sets, based on literature values only taken from studies of woody species, will be used for these comparisons.

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Chapter II. LITERATURE REVIEW

Introduction

Two general categories of nutrient uptake models, empirical and mechanistic models have been developed to study nutrient uptake by plant roots (Rengel 1993). Empirical models are based mainly on regressions as well as statistical means, often for practical use (Claassen and Steingrobe 1999). Mechanistic models, on the other hand, require an understanding of the mechanisms and a quantitative description of the phenomena (Rengel 1993). Mechanistic models are therefore useful to test the correctness of our knowledge of the phenomena (Claassen and Steingrobe 1999). Extrapolation of a verified mechanistic model is thus more reliable than that of an empirical model (Claassen and Steingrobe 1999). Another scientific application is the calculation of parameters that are difficult to obtain for either technical or economic reasons (Claassen and Steingrobe 1999). Model runs can also be used to identify topics that warrant further field or laboratory study. Finally, we can improve our understanding of the phenomena by exploring model behavior without conducting field trials (Barber 1995; Claassen and Steingrobe 1999).

Nutrient uptake by plant roots involves interdisciplinary studies: soil chemistry, soil physics, and plant physiology (Barber 1995). The typical mechanistic nutrient uptake model describes the supply of nutrients from bulk soil to root surfaces, root growth and morphology, and root uptake kinetics (Barber 1995).

The modeling of nutrient uptake started in the early 1960s. Bouldin (1961) and Olsen et al. (1962) proposed mathematical models to simulate diffusion of solutes through soils, which were used to explain phosphate movement and uptake. Nye and Spiers (1964) subsequently developed the partial differential equations used to describe simultaneous mass flow and diffusion for nutrient uptake by a unit length of root. Nye and Marriot (1969) defined boundary conditions for the equations and solved them numerically, while Baldwin et al. (1973), on the other hand, solved the equations analytically with steady state approximations. Their work became the foundation for mechanistic nutrient uptake models. Building on this base Claassen and Barber (1976), Nye and Tinker (1977), Barber and Cushman (1981), Claassen et al. (1986), Smethurst

and Comerford (1993b), Yanai (1994), Smethurst et al. (2004), and Comerford et al. (2006) proposed model revisions to cover the major sub-processes of nutrient uptake and to accommodate a variety of additional conditions. Current models have been successfully used in many areas of plant nutrition research.

In this review the soil and plant properties will be discussed first, followed by a mathematical description of the models and the use of sensitivity analysis to identify key parameters. Finally, a review of studies that have applied mechanistic nutrient uptake models to study woody species is presented. Because many parameters are involved, the symbols and their definitions are listed in Table 1.

Soil Characteristics

Nutrient availability in soils

Soil is a highly complex and heterogeneous system with many different components that provide plants with water and nutrients. Nutrients exist in the soil in gaseous, liquid, and solid forms. In this review only nutrients in liquid and solid forms will be discussed. Barber (1995) defined an available nutrient as "the nutrient present in a pool of ions in the soil and can move to the plant root during plant growth if the root is close enough". In the early development of mechanistic models, available nutrients were restricted to inorganic forms to simplify calculation (Barber 1995), but latter models such as SSAND are able to include nutrient from organic forms such as the mineralization of nitrogen (Comerford et al. 2006).

Transport processes

Interception, mass flow, and diffusion are the three components of nutrient movement to the root surface (Marschner 1995). Interception is used to describe the uptake of soil nutrients at the root interface when soil volume is displaced by root volume (Barber 1995). However, Tinker and Nye (2000) consider the concept of interception to be somewhat arbitrary and argued that it can be included in the diffusion component. Although conditions in the rhizosphere are sometimes different from those in the bulk soil (Marschner 1995), the contribution of interception to nutrient uptake is negligible for most nutrients (Barber 1995). Therefore, only mass flow and diffusion are considered to be responsible for movement of nutrients to the root surface in mechanistic modeling.

Table 1. List of symbols and definitions used in mechanistic nutrient uptake model equations.

Symbol	Definition
b	buffer power of nutrient
C	nutrient concentration in soil
C_{av}	average nutrient concentration in soil solution
C_L	nutrient concentration in soil solution
C_{L0}	nutrient concentration in soil solution at the root surface
C_{Li}	initial concentration of the nutrient in the soil solution
C_{min}	concentration in solution below which net influx ceases
C_s	nutrient concentration in soil solid phase
D	diffusion coefficient of solute
D_e	effective diffusion coefficient for the nutrient in the soil
D_L	diffusion coefficient of solute in water
E	nutrient efflux of plant roots
F	flux of solute
F_D	flux of solute by diffusion
F_M	flux of solute by mass flow
f_L	impedance factor of soil liquid-phase
f_s	impedance factor of soil solid-phase
I	net influx of solute per unit area of root surface
I_l	net influx of solute per unit length of root
I_{max}	maximum net influx at high nutrient concentrations
k	rate of root growth
K_m	Michaelis-Menten constant
L_0	initial root length
L_v	root length density
r	radial distance in soil from the root surface
r_0	mean root radius
r_1	half-distance between root axes
t	time
ΔU	the amount of nutrient uptake by root of unit length within a time period
U	the amount of nutrient uptake by root
U_p	the amount of nutrient uptake by root system within a time period predicted by PCATS
v	mean water influx
v_0	mean water influx at root surface
v_1	water influx at the distance r_1
x	distance
Δx	the extension of nutrient depletion zone in soil
α	root absorbing power
θ	volumetric soil moisture
ρ	soil bulk density

Mass flow

Mass flow is the convective transport of nutrients through the soil to the root surface by water flow as a result of transpiration (Barber 1995). The relative contribution of mass flow to nutrient uptake depends on the nutrient, plant species, plant age, and time of day (Marschner 1995). For example calcium and magnesium supplied to plants by mass flow is significant, but its contribution to potassium supply is negligible (Marschner 1995). The influx by mass flow (F_M) can be calculated by

$$F_M = vC_L \qquad [1]$$

where v is the mean water flux in soil driven by transpiration, and C_L is the nutrient concentration in the soil solution (Barber 1995).

Diffusion

Diffusion is the movement of nutrients from areas of high concentration to those of low concentration (Barber 1995). It is the main mechanism for at least phosphorus and potassium movement in the soil to plant roots (Marschner 1995). A depletion zone is produced when the concentration of nutrient is lowered near the root surface due to root absorption (Jungk and Claassen 1997). Diffusive flux F_D can be described by Fick's first law,

$$F_D = -D\frac{dC}{dx} \qquad [2]$$

where D is the diffusion coefficient of the nutrient in soil, C is the nutrient concentration in soil solution, and x is the distance. Diffusion in soils includes solute diffusion in soil solution and the surface diffusion on the soil solid phase (Tinker and Nye 2000). Thus the diffusion coefficient is calculated by

$$D = D_L f_L \theta dC_L/dC + D_L f_s \rho dS_s/dC \qquad [3]$$

where D_L is the diffusion coefficient of the solute in free solution, θ is the soil moisture, ρ is soil bulk density, f_L and f_s are liquid- and solid-phase impedance factors, respectively, and S_s is the amount of solute adsorbed on a unit weight of solid (Tinker and Nye 2000). The first part of equation [3] represents solute diffusion in solution, while the second part represents the surface diffusion on the soil solid phase. Usually only diffusion in soil solution is considered in the mechanistic nutrient uptake models, and the equation for the diffusion coefficient is reduced to

$$D = D_L f_L \theta dC_L/dC \qquad [4]$$

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With the addition of the equation for buffer power b

$$b = \frac{\mathrm{d}C}{\mathrm{d}C_L} \qquad\qquad [5]$$

equation [4] is rewritten as:

$$D_e = \frac{D_L f_L \theta}{b} \qquad\qquad [6]$$

where D_e is called the effective diffusion coefficient. It is also assumed that the liquid-impedance factor f_L is responsible for all the retarding effects from the solution and the solid phase during the process of diffusion (Tinker and Nye 2000) and mainly reflects the tortuosity, water density, and surface changes in the soil (Barber 1995).

Buffer power (b) reflects the relationship between nutrient concentration in the soil (C) and in the soil solution (C_L), and can be derived from sorption isotherms. Different sorption equations have been proposed. For example, $C = mC_L^n + a$, if the Freundlich equation is adopted, where a, m, and n are regression constants. Therefore, b can be obtained from such isotherm equations. Because the isotherm is usually non-linear, b is not constant when C_L changes.

The extension of the depletion zone can be calculated by

$$\Delta x = \sqrt{\pi D t} \qquad\qquad [7]$$

where Δx is the distance at which the decrease of concentration is 20% of the maximum decrease at the root surface, and t is time (Syring and Claassen 1995).

Simultaneous mass flow and diffusion

Mass flow and diffusion occur simultaneously to supply nutrients to plant roots and cannot be treated as separate processes. Nye and Spiers (1964) presented a partial differential equation (equation 8) to describe simultaneous mass flow and diffusion, and this equation became the foundation of the most mechanistic nutrient uptake models.

$$\qquad\qquad [8]$$

Plant Properties

Root morphology and growth

The root system that provides the plant with water and nutrients is very complex and dynamic. The basic mechanistic nutrient uptake models simplify the system by describing it with a few parameters. Root radius (r_0) is used to describe the root morphology. Root hairs play an

important role in some plants and the radius of the root hair is included if uptake by root hairs is considered. Initial root length (L_0) and root growth rate (k) are used to describe root growth. Two destructive harvests are usually required to obtain these parameters. Two mathematical methods are available to describe root growth rate. The linear way is to calculate k by

$$k = \frac{L_2 - L_1}{t_2 - t_1} \tag{9}$$

where t and L represent the time and root length at individual harvests, 1 and 2 representing the first and second harvest. The exponential way is to calculate k by

$$k = \frac{\ln L_2 - \ln L_1}{t_2 - t_1} \tag{10}$$

Half distance between root axes (r_1) is used to describe the influence of inter-root competition on nutrient uptake simulation. It is calculated by

$$r_1 = \sqrt{\frac{1}{\pi L_v}} \tag{11}$$

where L_v is the root length density (Barber 1995).

Nutrient uptake kinetics

Nutrient uptake mechanisms

The transport of nutrients across the cell membrane is the rate-limiting step when the nutrient supply is abundant (Williams and Yanai 1996). When nutrients arrive at the root surface, they are available for root absorption. The process can be divided into two types, passive and active uptake (Lodish et al. 2001). Passive uptake of nutrients refers to the transmembrane movement of nutrients without the consumption of energy (Lodish et al. 2001). It includes diffusion and facilitated diffusion along the concentration gradient between the inside and outside of the cell membrane (Lodish et al. 2001). Facilitated diffusion is the diffusion of ions with the help of ion channels or carrier proteins on the cell membrane (Lodish et al. 2001). For those nutrients whose concentration inside the cell is higher than outside, they will be transported across the membrane at the cost of energy, usually with the help of various membrane transporters (Lodish et al. 2001).

Marschner (1995) summarized the uptake isotherms and divided essential nutrients into three categories: (i) the uptake of potassium, phosphorus, nitrate, and sulfur usually depends on the

external nutrient concentration before it becomes saturated; (ii) the uptake of sodium, calcium, and magnesium also depends on the external concentration, but to a less extent, and there is no obvious pattern for leveling off; and (iii) boron uptake is by diffusion, in direct proportion to the external concentration. Recent studies of boron uptake by crop plants suggest that the mechanism of boron uptake is more complex. It involves both active and passive mechanisms, depending on the boron concentration in the soil solution at the root surface (Dannel et al. 2000; Pfeffer et al. 2001).

Modeling nutrient uptake kinetics

As early as the 1960s, root absorbing power (α) was used to connect the nutrient concentration in soil solution and the influx of nutrient into cells using the equation of Nye and Spiers (1964):

$$F = \alpha C_{L0} \qquad [12]$$

where C_{L0} is the nutrient concentration in soil solution at the root surface. α was assumed to be constant before the influx reaches its maximum (Nye and Spiers 1964; Nye and Marriott 1969; Baldwin et al. 1973; Nye and Tinker 1977). That is, influx increases linearly as the nutrient concentration in soil solution increases until the concentration reaches a critical point, above which the influx will be constant. If net influx per unit length of root (I_l) is used, the equation (Baldwin et al. 1973; Nye and Tinker 1977) is transformed to

$$I_l = 2\pi r_0 \alpha C_{L0} \qquad [13]$$

where r_0 is the root radius.

Reflecting advances in the understanding of cell biology, the mechanism of active uptake was incorporated into the models by Claassen and Barber (1976). Active uptake is described by the Michaelis-Menten equation:

$$I = \frac{I_{max}(C_{L0} - C_{min})}{K_m + C_{L0} - C_{min}} \text{ or } I = \frac{I_{max}C_{L0}}{K_m + C_{L0}} - E \qquad [14]$$

where I is the nutrient influx per unit area of root surface, I_{max} is the maximal influx at high C_L, K_m is the Michaelis-Menten constant, C_{min} is the solution concentration at which influx equals to efflux, and E is the efflux of ions from roots into solution.

The relationship between C_{L0} and I described by Michaelis-Menten equation indicates that the root absorbing power constantly changes as C_{L0} changes. To incorporate active uptake

kinetics in their model, Smethurst and Comerford (1993b) used a variable root absorbing power (equation 15).

$$\alpha = \frac{I_{max}}{K_m + C_{L0} - C_{min}} \qquad [15]$$

Modeling Approaches

Over the past four decades different mechanistic nutrient uptake models have been developed to simulate nutrient uptake. Usually, these models consist of three basic components (Rengel 1993): (i) solute movement in the soil toward plant roots described by the continuity equation (equation 8); (ii) nutrient uptake kinetics described by the Michaelis-Menten equation (equation 14); (iii) nutrient uptake as a result of root growth and inter-root competition by introducing root growth and morphology parameters. Two categories of models have evolved, steady state and transient models (Tinker and Nye 2000). NST 3.0 is an example of a transient model with a numerical solution, while SSAND and PCATS are steady state models.

The basic principles of NUTRIENT UPTAKE and NST 3.0

Transient models utilizing numerical solutions are a well established approach to mechanistic nutrient uptake models (Tinker and Nye 2000). The Barber-Cushman model is a well-known and widely-used model in this category. NUTRIENT UPTAKE model and NST 1.0 are the personal computer version of the Barber-Cushman model (Oates and Barber 1987; Claassen et al. 1968). NST 3.0 is an improved version of NST 1.0. In this section, the principles of NUTRIENT UPTAKE model are presented, followed by a brief introduction to NST 3.0.

The Barber-Cushman model is largely based on the work by Nye and Marriot (1969). Nye and Marriot (1969) revised the continuity equation proposed by Nye and Spiers (1964) (see equation 8) to describe the flux of nutrient in the soil to the root surface with the nutrient concentration in soil solution (C_L):

$$\frac{1}{r}\frac{\partial \left(rD\frac{\partial C_L}{\partial r} + \frac{v_0 r_0 C_L}{b}\right)}{\partial r} = \frac{\partial C_L}{\partial t} \qquad [16]$$

where v_0 is the water flux at the root surface, r is the radial distance from the root, and t is time. Nye and Marriot (1969) defined boundary conditions and solved this equation numerically.

Summarizing the work by Claassen and Barber (1976) and Cushman (1979a; 1979b), Barber and Cushman (1981) suggested new boundary conditions for the equation [16] to include inter-root competition for nutrients:

(1) Inner boundary condition

$$t > 0, r = r_0, F = Db\frac{\partial C_L}{\partial r} + v_0 C_L = \frac{\alpha C_L}{1 + \alpha C_L/I_{max}} - E \qquad [17]$$

where $(\frac{\alpha C_L}{1+\frac{\alpha C_L}{I_{max}}} - E)$ is a transformation of the equation [14].

(2) Outer boundary condition:

If there is no inter-root competition,

$$t > 0, r = r_1, C_L = \text{constant} \qquad [18]$$

If there is inter-root competition,

$$t > 0, r = r_1, F = Db\frac{\partial C_L}{\partial r} + v_1 C_L = 0 \qquad [19]$$

where v_1 is the water influx at a distance of r_1.

The new boundary conditions incorporated inter-root competition as well as Michaelis-Menten kinetics. When solved numerically, the enhanced mechanistic model evolved into Barber-Cushman model. In 1983 Itoh and Barber developed a submodel to the Barber-Cushman model to include nutrient uptake by root hairs.

In 1986 Claassen et al. published NST 1.0 model. In 1987 Oates and Barber published NUTRIENT UPTAKE model. Both were based on the Barber-Cushman model. Later Claassen and his colleagues developed NST 2.0 and NST 3.0, which were not published in a journal (Claassen, N. Personal communication. 2009, 31 July). NST 3.0 incorporates the Freundlich isotherm into the model so that the buffer power (b) changes as the nutrient concentration in soil solution changes (Steingrobe et al. 2000).

The basic principles of COMP8, SSAND, and PCATS

Steady state models are the other standard method in mechanistic nutrient uptake modeling (Tinker and Nye 2000). Baldwin et al. (1973) and Nye and Tinker (1977) proposed the key equations in 1970s. Based on their work, Smethurst and Comerford (1993b) developed a computer model, COMP8 (Competition model version 8), which was able to calculate nutrient uptake between two competing and contrasting root systems. SSAND was a revision and

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expansion of COMP8 by Comerford et al. (2006). Its main improvements lie in the functions of predicting nutrient uptake as influenced by mycorrhizae and simulation of fertilization effects (Comerford et al. 2006). Based on COMP8 and an earlier version of SSAND, another steady state model, PCATS was developed to simulate nutrient uptake by a single species by Smethurst et al. (2004). In this section, the principle of steady state models is briefly described; and the features of COMP8, SSAND and PCATS are introduced.

Based on the continuity equation by Nye and Spiers (1964) (see equation 8), Baldwin et al. (1973) and Nye and Tinker (1977) proposed the key equations of the concentration profile around the root as well as the average concentration for use in a steady state model.

$$\frac{C_{Lr}}{C_{L0}} = \frac{\alpha}{v_0} + \left[1 - \frac{\alpha}{v_0}\right] \left(\frac{r}{a}\right)^{-\left(\frac{r_0 v_0}{bD}\right)}$$

[20]

where C_{Lr} is the nutrient concentration in soil solution at the distance r from the root.

By representing the average concentration across the depletion zone with C_{av}, the relationship between C_{av} and C_{L0} can be obtained by

$$\frac{C_{av}}{C_{L0}} = \frac{\alpha}{v_0} + \left(1 - \frac{\alpha}{v_0}\right)\left(\frac{2}{2 - \frac{r_0 v_0}{bD}}\right)\frac{\left(\frac{r_1}{r_0}\right)^{\left(2 - \frac{r_0 v_0}{bD}\right)} - 1}{\left(\frac{r_1}{r_0}\right)^2 - 1}$$

[21]

Because the amount of nutrient uptake ΔU during the time period Δt is given by

$$\Delta U = 2\pi r_0 L_v \alpha C_{L0} \Delta t$$

[22]

ΔU can be calculate by equation [23] and [24]. That is

$$\Delta U = 2\pi r_0 L_v \alpha \Delta t \frac{C_{av} v_0}{\alpha + (v_0 - \alpha)\left(\frac{2}{2 - \frac{r_0 v_0}{bD}}\right)\frac{\left(\frac{r_1}{r_0}\right)^{\left(2 - \frac{r_0 v_0}{bD}\right)} - 1}{\left(\frac{r_1}{r_0}\right)^2 - 1}}$$

[23]

At time interval Δt_1, $C_{av1} = C_{Li}$. Therefore the new C_{av2} can be calculated from the uptake at time interval Δt_2, and C_{La2} can be calculated from C_{av2}. This approach allows any time period to be represented (Tinker and Nye 2000). Finally, the total amount of nutrient uptake can be obtained by summing ΔU at each time interval.

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Smethurst and Comerford (1993b) developed COMP8 based on the above equation and another equation dealing with the competition between two root systems, with the improvements that allow for (i)" a depletion zone that increases with time until it reaches the no-transfer boundary, (ii) an adjustment in concentration to reflect newly encountered solutes in the depletion zone, (iii) a variable root absorbing power α (see equation 15) to describe Michaelis-Menten uptake kinetics, and (iv) a routine to account for the competition between two root systems". Two verification studies with slash pine and weeds were also conducted in the same year (Smethurst and Comerford 1993a; Smethurst et al. 1993). However, this model has had little use since 1993 because it was inadequate under some conditions possibly due to the inability of the model to describe some components of the soil-root system such as root length development, changing moisture contents, and the nutrient input from mineralization (Smethurst and Comerford 1993b).

Based on COMP8, SSAND included several new functions allowing simulation of nutrient uptake by roots under a variety of conditions such as mycorrhizal roots, fertilization, changing soil water content, nutrients from different soil horizons, and dynamic mineralization rates (Comerford et al. 2006). It includes sub-routines to calculate the nutrient demand for a target plant growth, so that it can provide a recommendation on fertilization by comparing the predicted uptake and demand.

Similar to SSAND, PCATS is able to simulate nutrient uptake by mycorrhizae as well as uptake influenced by fertilization (Smethurst et al. 2004). However, it can only predict nutrient uptake by one species. It also uses an analytical solution similar to COMP8 and SSAND, but further simplifies the calculation by running on a fixed daily time-step (Smethurst et al. 2004).

Assumptions for the mechanistic models

A number of specific assumptions underlie the models.

- The soil is homogeneous and isotropic (Rengel 1993).
- Nutrients move to the root by a combination of mass flow and diffusion (Barber 1995).
- Roots are smooth cylinders and the nutrient absorbing power is the same over all the cylinders (Barber 1995).

- Mycorrhizae, root hairs, root exudates, or microbial activity on the root surface do not influence nutrient flux (Barber 1995).
- Nutrient uptake can be described by Michaelis-Menten kinetics and the kinetics parameters do not change over time (Barber 1995).
- Influx is independent of the rate of water absorption (Barber 1995)
- For NST 3.0, the soil moisture is essentially constant (Barber 1995). The roots are distributed evenly in the whole soil volume, and no allowance is given for a changing distance among roots as roots grow (Claassen and Steingrobe 1999); A root segment can exploit only a limited volume of soil, and the root is at the center of this cylinder (Claassen and Steingrobe 1999).
- For SSAND and PCATS, Roots are assumed to be parallel and distributed regularly throughout the soil volume (Baldwin 1973).

Comparison of the two major categories of mechanistic models

Usually transient state models with a numerical solution are considered to be more accurate than steady state models (Smethurst and Comerford 1993b; Yanai 1994). Numerical methods are those that "iteratively solve a system of simultaneous equations developed from approximations of the differential equation for solute transport" (Smethurst and Comerford 1993b). "The steady state approach assumes that the concentration profile around the root can be considered to be in a steady state" (Yanai 1994), which is usually attained after long periods of time (Nye and Spiers 1964). Since natural phenomena are transient, the results obtained using this approach may not be as accurate as the transient state model.

The major advantage of a steady state model over a transient state model lies in "the independence of the mathematical solution to previous condition" during calculation (Yanai 1994) so that steady state models are able to respond to real-time changes in parameters. Transient state models using a numerical solution are also called "deterministic" models (Claassen and Steingrobe 1999) because the simulation does not accept time-varying input (Yanai 1994). For example, soil moisture is not allowed to change during the calculation, though it is unrealistic to think that soil moisture would remain constant in the field.

Current study on NST 3.0, SSAND, and PCATS

As a transient model utilizing a numerical solution, NST 3.0 has been used widely to predict uptake of nutrients by various crop species (Sadana and Claassen 2000; Satnam and Sadana 2002; Samal et al. 2003; Sadana et al. 2005; Pypers et al. 2006). However, no studies on woody species utilizing this model have been conducted.

Smethurst and Comerford (1993b) verified the ability of COMP8 to predict a one-species scenario by comparing its responses with those of the NUTRIENT UTPAKE model. They also published the verification of COMP8 by predicting potassium and phosphorus uptake by slash pine in competition with weeds using both pot and field studies (Smethurst and Comerford 1993a; Smethurst et al. 1993). In the pot study, the model provided a good representation of potassium and phosphorus uptake by pines and weeds under high nutrient concentration treatments, but performed poorly under low nutrient concentration treatments (Smethurst and Comerford 1993a). In the field study, the model predicted the phosphorus and potassium uptake by pines adequately, but significantly over predicted uptake of both nutrients by weeds (Smethurst et al. 1993). Ibrikci et al. (1994) studied phosphorus uptake by Bahiagrass with COMP8. The prediction matched the observation for 18-day-old plants growing in Ap, E, and Bh horizons, but a low level of agreement was found at 90 days for plants growing in Ap and E horizon soils, both of which were known to be of low phosphorus supply (Ibrikci et al. 1994). Four years later, Ibrikci and his colleagues (1998) found that the nitrogen uptake predicted for COMP8 was 38% to 44% lower than that observed by field-grown corn (Ibrikci et al. 1998). The potential error of adopting an I_{max} value from the literature and COMP8's inability to include contributions from root hairs and nitrogen mineralization were suggested by Ibrikci et al. (1994) as the reasons for their underestimates.

SSAND was published in 2000 (Li and Comerford 2000); the authors verified it by predicting phosphorus uptake by 1-yr loblolly pine growing in southeastern Georgia and Florida (Comerford et al. 2006). Borges-Gómez et al. (2008) used SSAND to predict potassium requirement by habanero pepper in Yucatán, Mexico. But they used SSAND as a tool for management and did not compare the model predictions to any observations of uptake. Singh (2008) investigated the uptake of nitrogen, phosphorus, and potassium by hybrid poplar and weeds in both the lab and field using SSAND. The disagreement between the simulated and

observed uptake was significant except for the simulation of nitrogen uptake by hybrid poplar in the control field site (Singh 2008). Only one paper is available for the model PCATS. The authors verified the model by comparing the PCATS estimates of uptake to these provided by NUTRIENT UPTAKE model (Smethurst et al. 2004).

To summarize, the differences between NST 3.0, SSAND, and PCATS are not well understood in terms of predictive accuracy and model behavior. The different solution methods used in the models may lead to different simulations. Reported research to date related to the use of SSAND and PCATS is limited. Agreement between the predictions of their predecessor model, COMP8, and observations was not good under some situations such as low nutrient supply scenarios (Smethurst and Comerford 1993a). Although NST 3.0 performed well with crop species, no tests have been done with woody species. Because no study has been conducted to compare the efficacy of the three models, it would be beneficial to evaluate the three models by comparing the predictions with observations using multiple datasets representing various situations taken from the literature.

Sensitivity Analysis of Mechanistic Nutrient Uptake Models

The traditional sensitivity analysis can also be called a one dimensional sensitivity analysis. This approach was first used to by Silberbush and Barber in 1983 to show the influence of different parameters on model simulations. It was accomplished by changing a single model input parameter while keeping the others constant (Silberbush and Barber 1983). By plotting the change ratio of the parameters compared to their original values on the horizontal axis, and the predicted uptake to the original prediction on the vertical axis, it is possible to evaluate the importance of each parameter by the slope of the line on the graph. This procedure has been largely followed in all subsequent analysis. Although Claassen and Steingrobe (1999) proposed to treat initial soil solution concentration (C_{Li}) and buffer power (b) together in the analysis because the two parameters are related to each other, the principle is the same.

Yanai proposed the idea of multiple dimensional sensitivity analysis in 1994 and did several two dimensional sensitivity analyses. Two years later Williams and Yanai conducted a multiple dimensional sensitivity analysis using a simplified steady state model to simulate nutrient uptake by a unit length of root (Williams and Yanai 1996). Because the model they used did not take root growth and inter-root competition into account, it contained 7 parameters, while a typical

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mechanistic nutrient uptake model has 11 parameters. By changing each parameter at 4 levels, 16,384 parameter datasets were created. Using ANOVA, they found up to four-way interactions among the parameters with C_{av}, I_{max}, D_e, and r_0 exerting the most significant influences on the simulations (Williams and Yanai 1996). They then represented each of 5 parameters (these 4 parameters plus water influx into roots) at 5 levels and plotted the response surface using graphs (Williams and Yanai 1996). The response surfaces developed using this method indicated clear relationships between the selected parameters. For example, the most influential parameters depend on the concentration of nutrients supplied by soil processes (Williams and Yanai 1996). When the concentration is low, the soil parameters dominate the uptake process. When the concentration is high, the parameters representing the ability of the plant root to take up nutrients, such as I_{max} and r_0, will determine how much nutrient is taken up (Williams and Yanai 1996).

Therefore, the multiple dimensional sensitivity analysis is a powerful tool in helping us understand model behavior under various situations. However, since the simplified mechanistic model used by Williams and Yanai (1996) did not include inter-root competition and root growth, using this method to analyze NST 3.0, SSAND, and PCATS with the key parameters C_{av}, I_{max}, D_e, r_0, plus the parameters of root growth and inter-root competition would provide a more complete evaluation of the model behaviors and explore the potential differences between the three models more thoroughly.

Nutrient Uptake Modeling of Woody Species

Gillespie and Pope (1990) used the Barber-Cushman model combined with a model on rhizosphere acidification to study phosphorus uptake by black locust. It is the first study to employ a minimalistic mechanistic nutrient uptake model to study a woody species. Gillespie and Pope (1990) found that the predictions matched the observations well if the influence of rhizosphere acidification was considered. In the same year, Van Rees et al. (1990) reported a study on potassium uptake by slash pine with both the Barber-Cushman and the Baldwin-Nye-Tinker models. The Baldwin-Nye-Tinker model (BNTM) was developed by Baldwin et al. in 1973 and became the foundation for COMP8 in 1993. Van Rees et al. (1990) found that the prediction by BNTM was 5% higher than that by the Barber-Cushman model and that both models only worked well under situations treated with fertilizers.

In collaboration with S. A. Barber, Kelly and Barber (1991) reported the magnesium uptake kinetics parameters of loblolly pine as well as the influence of seedling age on these parameters. In the following year, Kelly et al. (1992) verified the use of the Barber-Cushman model on phosphorus and potassium uptake by loblolly pine seedlings, but the simulated uptake of magnesium was substantially underestimated. From the mid 1990s to the early 2000s, Kelly and his coworkers used NUTRIENT UPTAKE model to study the uptake of several macro-nutrients by various tree species under different growing treatments (Kelly et al. 1995; Kelly et al. 2000; Kelly and Kelly 2001; Kelly et al. 2001; Adam et al. 2003; Kelly and Ericsson 2003). The research largely focused on the influence of environmental factors and plant growth on parameter values, such as the seasonal dynamics of soil supply capacities (Kelly et al. 1995) and the uneven growth of roots during a growing season (Kelly et al. 2001). Some limitations of NUTRIENT UPTAKE model were also pointed out, such as the fixed root growth rate (Kelly et al. 2001) and the inability to include the contributions of decomposition and mineralization during the simulation (Kelly and Ericsson 2003). Adam et al. (2003) also used these parameters and the established methodology as tools to study the influence of temperature on uptake kinetics (Adam et al. 2003).

Unlike the Barber-Cushman model, the steady state model has been constantly revised since 1990s, and most of the studies were conducted with woody species. Because COMP8, Yanai's model in 1994, SSAND, and PCATS are important achievements in the development of the steady state model, and they are discussed in the section discussing the current studies of SSAND and PCATS, these studies are not repeated here. Yanai (2003) used the steady state mechanistic model she proposed in 1994 to calculate the nutrient concentration differences between rhizosphere and bulk soil in a Norway spruce stand. She found that in contrast to the model calculation, the observed nutrient concentrations in the rhizosphere were generally higher than those in bulk soil (Yanai et al. 2003).

Representative ranges for parameters needed conduct a multiple dimensional sensitivity analysis are presented in Tables 2, 3, and 4 and list values from the literature for nutrient uptake kinetics, soil supply, and root growth parameter.

Table 2. Nutrient uptake kinetics parameters for a variety of woody species taken from the literature.

Nutrient	Species	Common name	I_{max} $\mu mol\ cm^2\ s^{-1}$	K_m $\mu mol\ cm^{-3}$	C_{min} $\mu mol\ cm^{-3}$	Source
NH_4-N	*Populus* sp.	hybrid poplar	0.000004	0.049	0.001	(Singh 2008)
	Picea glauca	white spruce	0.0000207	0.20568		(Hangs et al. 2003)
	Populus tremuloides	aspen	0.00001254	0.21712		(Hangs et al. 2003)
NO_3-N	*Populus* sp.	hybrid poplar	0.0000034-0.0000285	0.093-0.712	0.001	(Kelly and Ericsson 2003)
	Acer rubrum	red maple	0.0000157-0.00005908	0.204-0.523	0.001	(Kelly et al. 2000)
	Acer rubrum	red maple	0.0000195-0.0000318	0.000088-0.00019	0.000018-0.000066	(Adam et al. 2003)
	Acer rubum	red maple	0.0000309	0.32	0.001	(Kelly et al. 2001)
	Picea glauca	white spruce	0.0000045	0.34451		(Hangs et al. 2003)
	Populus tremuloides	Aspen	0.00000581	0.3365		(Hangs et al. 2003)
K	*Populus* sp.	hybrid poplar	0.0000176	0.0269	0.003	(Kelly and Ericsson 2003)
	Populus sp.	hybrid poplar	0.00000266	0.034	0.001	(Singh 2008)
	Acer rubrum	red maple	0.0000038	10.46	0.003	(Kelly and Kelly 2001)
	Pinus elliottii var. *elliottii*	slash pine	0.00000361	0.029	0.001	(Van Rees et al. 1990)
	Pinus elliottii var. *elliottii*	slash pine	0.00000361	0.029	0.001	(Van Rees and Comerford 1990)
	Pinus taeda	loblolly pine	0.0000014	0.03	0.001	(Kelly et al. 1992)
	Pinus taeda	loblolly pine	0.00000365	0.0237	0.0002	(Kelly et al. 1995)
P	*Populus* sp.	hybrid poplar	0.00000151	0.00087	0.001	(Kelly and Ericsson 2003)
	Populus sp.	hybrid poplar	0.00000113	0.038	0.001	(Singh 2008)
	Acer rubrum	red maple	0.00000549	15.02	0.001	(Kelly and Kelly 2001)
	Pinus elliottii var. *elliottii*	slash pine	0.000000643	0.00545	0.0002	(Smethurst and Comerford 1993a)
	Pinus taeda	loblolly pine	0.000000268	0.016	0.0006	(Kelly et al. 1992)
	Pinus taeda	loblolly pine	0.00000064	0.00545	0	(Comerford et al. 2006)
	Robinia pseudoacacia	black locust	0.0000017	0.0018	0.0007	(Gillespie and Pope 1990)
Mg	*Pinus taeda*	loblolly pine	0.000000112	0.00858	0.001	(Kelly and Barber 1991)
	Pinus taeda	loblolly pine	0.000000079	0.00869	0.001	(Kelly and Barber 1991)
	Pinus taeda	loblolly pine	0.000000129	0.00983	0.001	(Kelly and Barber 1991)
	Pinus taeda	loblolly pine	0.000000129	0.00983	0.001	(Kelly et al. 1992)

Table 3. Soil supply parameters from studies of a variety of woody species.

Nutrient	C_{Li} μmol ml^{-1}	b	D_e cm^2 s^{-1}	Plant name	Source
NH$_4$-N	0.0037-0.714			hybrid poplar	(Singh 2008)
	0.001-0.075	4.9-209.3	0.000000015-0.00000131	multiple species	(Kelly and Mays 1999)
	0.052-0.215		0.0000064-0.000015	Norway spruce	(Yanai et al. 2003)
NO$_3$-N	0.0761-2.31	1.14-1.98	0.000000684-0.000113	hybrid poplar	(Kelly and Ericsson 2003)
	0.047-10.714			hybrid poplar	(Singh 2008)
	0.002-2.33	0.04-69.09	0.000000191-0.0002	multiple species	(Kelly and Mays 1999)
	0.51	1.35	0.0000632	red maple	(Kelly et al. 2001)
K	0.124-0.132			cottonwood	(Wang et al. 2004)
	0.0963-0.519	1.4-5.095	0.000000263-0.000000994	hybrid poplar	(Kelly and Ericsson 2003)
	1.432-3.529			hybrid poplar	(Singh 2008)
	0.27	10.55	0.00000329	loblolly pine	(Kelly et al. 1992)
	0.99-8.54	0.16-1.19	0.000000664-0.00000635	loblolly pine	(Kelly et al. 1995)
	0.018-0.561			multiple species	(Kelly and Mays 1999)
	0.028-0.142		0.0000048-0.000017	Norway spruce	(Yanai et al. 2003)
	0.112	20	0.000000358	red maple	(Kelly and Kelly 2001)
	0.13	7.02	0.00000171	red maple	(Kelly et al. 2001)
	0.035-0.06	3.00-3.44	0.000000291-0.000000628	slash pine	(Van Rees et al. 1990)
	0.093-0.203	3.64-6.26	0.00000002-0.000000104	slash pine	(Van Rees and Comerford 1990)
	0.0382-0.338	0.55-2.13	0.00000019-0.00000128	slash pine	(Smethurst and Comerford 1993a)
	0-0.36	0.7-4.3		slash pine	(Smethurst et al. 1993)
P	0.00161-0.00484			black locust	(Gillespie and Pope 1990)
	0.0287-0.0339			cottonwood	(Wang et al. 2004)
	0.0021-0.0388	15.41-180.5	0.000000003-0.000000041	hybrid poplar	(Kelly and Ericsson 2003)
	0.016			hybrid poplar	(Singh 2008)
	0.19	5.84	0.000000817	loblolly pine	(Kelly et al. 1992)
	0.0032			loblolly pine	(Comerford et al. 2006)

Table 3. (Continued)

Nutrient	C_{Li} $\mu mol\ ml^{-1}$	b	D_e $cm^2\ s^{-1}$	Plant name	Source
P	0.001-0.01	84.5-1451.5	0.0000000091-0.000000029	multiple species	(Kelly and Mays 1999)
	0.001	199	0.0000000203	red maple	(Kelly and Kelly 2001)
	0.001	166.8	0.0000000143	red maple	(Kelly et al. 2001)
	0.0226-1.21	0.23-0.85	0.00000019-0.0000013	slash pine	(Smethurst and Comerford 1993a)
	0-0.29	0.7-1520		slash pine	(Smethurst et al. 1993)
Ca	0.644-0.706			cottonwood	(Wang et al. 2004)
	0.019-0.599			multiple species	(Kelly and Mays 1999)
	0.004-0.009		0.000019-0.000067	Norway spruce	(Yanai et al. 2003)
Mg	0.560-0.609			cottonwood	(Wang et al. 2004)
	1.35	1.32	0.000000145	loblolly pine	(Kelly et al. 1992)
	0.012-0.37			multiple species	(Kelly and Mays 1999)
	0.018-0.047		0.0000017-0.000006	Norway spruce	(Yanai et al. 2003)
S	0.028-0.051		0.0000026-0.000009	Norway spruce	(Yanai et al. 2003)

Table 4. Root growth parameters from a variety of woody species and the mean water flux at the root surface taken from the literature.

Plant name	L_0 cm	L_v cm cm^{-3}	r_0 cm	r_1 cm	k cm s^{-1}	v_0 cm s^{-1}	Source
hybrid poplar	1094		0.02	0.573-0.664	0.000347-0.00113	0.000000746	(Kelly and Ericsson 2003)
hybrid poplar		0.001-11.88	0.01-0.03			0.00000195	(Singh 2008)
box elder			0.0675				(Comas et al. 2002)
red maple			0.035-0.0397				(Adam et al. 2003)
red maple	3842-16179		0.028-0.042				(Kelly et al. 2000)
red maple	1696		0.044	0.99	0.000475	0.00000517	(Kelly et al. 2001)
sugar maple			0.0685				(Comas et al. 2002)
white spruce			0.041				(Hangs et al. 2003)
Norway spruce			0.05	0.36-0.55		0.0000016-0.0000021	(Yanai et al. 2003)
jack pine			0.039				(Hangs et al. 2003)
Eastern hemlock			0.0783				(Comas et al. 2002)
slash pine	16.6-31.6		0.036-0.06	1.39-3.15	0.000012-0.000184	0.00000379	(Van Rees et al. 1990)
slash pine		0.1-0.3	0.0234-0.0932			0.0000032	(Smethurst and Comerford 1993a)
slash pine	11.9-41.3		0.027-0.046	0.62-2.59	0.000064-0.000455	0.00000223-0.00001035	(Van Rees and Comerford 1990)
loblolly pine	10-517.3		0.043-0.052	2.47-6.02	0.00004-0.00013	0.000000566	(Kelly et al. 1995)
loblolly pine	285		0.035	2	0.000162	0.000000566	(Kelly et al. 1992)
loblolly pine		0.4	0.04			0.000002	(Comerford et al. 2006)
Virginia pine			0.0741				(Comas et al. 2002)
cottonwood	301.1						(Wang et al. 2004)
aspen			0.043				(Hangs et al. 2003)
white oak			0.0504				(Comas et al. 2002)
red oak			0.0605				(Comas et al. 2002)
black locust				0.941		0.000000001	(Gillespie and Pope 1990)

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Chapter III. NUTRIENT UPTAKE ESTIMATES FOR WOODY SPECIES AS DESCRIBED BY THE NST 3.0, SSAND, AND PCATS MECHANISTIC NUTRIENT UPTAKE MODELS

Abstract

Mechanistic nutrient uptake models have been developed based on the principles of nutrient movement in the soil, nutrient uptake kinetics, and root growth and morphology. There are two major categories of mechanistic models, transient state models with a numerical solution and steady state models. NST 3.0 belongs to the former set of models, while SSAND and PCATS belong to the latter. Because the different approaches to solution between transient and steady state models may lead to different simulation results, and studies using the three models to assess woody species are limited, it would be useful to evaluate the three models by comparing model predictions based on common data sets taken from the literature against the observed measurements. Therefore, the objectives of this study are to: (i) compare the predictions of uptake by the NST 3.0, SSAND, and PCATS models for a suite of nutrients against experimentally measured values, (ii) compare the behavior of the three models using a one dimensional sensitivity analysis; and (iii) compare and contrast the behavior of NST 3.0 and SSAND using a multiple dimensional sensitivity analysis. The predictions of nutrient uptake by the three models using the same data set were diverse, indicating a need to reexamine model structure. Further studies using representative datasets are also needed so that the predictive accuracy of each model can be evaluated. Both types of sensitivity analyses suggested that the effect of soil moisture on simulation can be influential when nutrient concentration in the soil solution (C_{Li}) is low. One dimensional sensitivity analysis also revealed that I_{max} negatively influenced estimates of nutrient uptake in the SSAND and PCATS models. Further analysis indicated that this phenomenon was related to the low nutrient supply ability of the soils. The predictions of SSAND under low-nutrient-supply scenarios are generally lower than these of NST 3.0 (the greatest underestimate was 100%). We suspect that both of these results are artifacts of the steady state models and further studies to improve them are required. Modeling

the influence of rhizospheric effects warrants more emphasis because of the longer growth periods and low nutrient supply situations more typical related to woody species.

Introduction

Mechanistic modeling of nutrient uptake started in the early 1960s when Bouldin (1961) and Olsen et al. (1962) proposed mathematical models to simulate the diffusion of solutes through soils. Models of plant uptake based on the seminal efforts by Nye and Spiers (1964), Nye and Marriot (1969), and Baldwin et al. (1973), and advanced by the subsequent work of Claassen and Barber (1976), Nye and Tinker (1977), Barber and Cushman (1981), Claassen and Steingrobe (1999), and Steingrobe et al. (2000), are becoming important research tools. Mechanistic modeling took a significant step forward with advent of the personal computer as reflected in the work of Oates and Barber (1987), Smethurst and Comerford (1993b), Yanai (1994), Smethurst et al. (2004), and Comerford et al. (2006). Usually, these models consist of three basic components represented by a set of equations that describe (Rengel 1993): (i) solute movement in the soil toward plant roots using the continuity equation that expresses "the change in mass of a substance in a small volume over a small time" (Tinker and Nye 2000); (ii) nutrient uptake kinetics using the Michaelis-Menten equation; and (iii) nutrient uptake as a result of root growth and inter-root competition through the use of root growth and morphology parameters. Depending on the way in which the continuity equation is solved, two major categories of models have evolved, steady state or transient state models (Tinker and Nye 2000). NST 3.0 is an example of a transient state model with a numerical solution, while SSAND and PCATS are steady state models.

Research on several crop species has demonstrated that the predictions of these mechanistic models generally match the observed uptake under situations in which the soil and plant conditions are relatively constant (Barber 1995). However, results with woody species have been more variable (Gillespie and Pope 1990; Van Rees et al. 1990; Smethurst and Comerford 1993b).

One way to evaluate the models is by comparing model predictions with measured values. A second approach is the use of sensitivity analysis. The traditional way to conduct a sensitivity analysis in the modeling context is by changing a single input parameter in the model while keeping the others constant (Silberbush and Barber 1983). Williams and Yanai (1996) suggested this method be called a one dimensional sensitivity analysis. However, because "the relative

importance of parameters defined this way can depend strongly on the values of the other parameters", Williams and Yanai (1996) developed a multiple dimensional sensitivity analysis in order to study model behavior across a broad range of possible parameter values.

Differences between NST 3.0, SSAND, and PCATS are not well understood in terms of predictive accuracy and model behavior. The different development methods used in the models may lead to different simulations. Research to date related to the use of SSAND and PCATS is limited. Agreement between the uptake predictions of their predecessor model, COMP8, and observed values were not good in low nutrient supply scenarios (Smethurst and Comerford 1993a). Although NST 3.0 has performed well with crop species, no tests have been done with woody species. Because no study has been conducted to compare the efficacy of the three models, it would be beneficial to evaluate the three models by comparing model predictions with nutrient uptake observations using multiple datasets representing various situations taken from the literature and by conducting sensitivity analyses.

Therefore, the objectives of this study are to: (i) compare the predictions of uptake by the NST 3.0, SSAND, and PCATS models for a suite of nutrients against experimentally measured values, (ii) compare the behavior of the three models using a one dimensional sensitivity analysis; and (iii) compare and contrast the behavior of NST 3.0 and SSAND using the multiple dimensional sensitivity analysis approach of Williams and Yanai (1996).

Material and Methods

Basic principles and model assumptions

Mechanistic nutrient uptake models are very complex nonlinear models. They were developed based on understanding from multiple disciplines including soil chemistry, soil physics, and plant physiology and improved constantly by the advances in these fields. NST 3.0, SSAND, and PCATS belong to two major categories of mechanistic models, and represent the current state of the art. In order to make a successful comparison, it is necessary to review the basic principles and assumptions of these mechanistic models. Table 5 lists the primary symbols and parameters that are used in the mechanistic models described in this paper.

A number of both general and specific assumptions underlie the models.

- The soil is homogeneous and isotropic (Rengel 1993).

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Table 5. List of symbols and definitions used in the NST 3.0, SSAND, and PCATS mechanistic nutrient uptake model equations.

Symbol	Definition
b	buffer power of nutrient
C	nutrient concentration in soil
C_{av}	average nutrient concentration in depletion zone
C_L	nutrient concentration in soil solution
C_{L0}	nutrient concentration in soil solution at the root surface
C_{Li}	initial concentration of the nutrient in the soil solution
C_{min}	concentration in solution below which net influx ceases
D	diffusion coefficient of solute
D_e	effective diffusion coefficient for the nutrient in the soil
D_L	diffusion coefficient of solute in water
E	nutrient efflux of plant roots
F	flux of solute
F_D	flux of solute by diffusion
F_M	flux of solute by mass flow
f	impedance factor or tortuosity factor
I	net influx of solute
I_{max}	maximum net influx at high nutrient concentrations
k	rate of root growth
K_m	Michaelis-Menten constant
L_0	initial root length
L_v	root length density
r	radial distance in soil from the root surface
r_0	mean root radius
r_1	half-distance between root axes
t	time
U	the amount of nutrient uptake by a root or root systems
v	mean water influx
v_0	mean water influx at root surface
v_1	water influx at the distance r_1
α	root absorbing power
θ	volumetric soil moisture

- Nutrients move to the root by a combination of mass flow and diffusion (Barber 1995).
- Roots are smooth cylinders and the nutrient absorbing power is the same over all the cylinders (Barber 1995).
- Mycorrhizae, root hairs, root exudates, or microbial activity on the root surface do not influence nutrient flux (Barber 1995).
- Nutrient uptake can be described by Michaelis-Menten kinetics and the kinetics parameters do not change over time (Barber 1995).
- Influx is independent of the rate of water absorption (Barber 1995)
- For NST 3.0, the soil moisture is essentially constant (Barber 1995). The roots are distributed evenly in the whole soil volume, and no allowance is given for a changing distance among roots as roots grow (Claassen and Steingrobe 1999); A root segment can exploit only a limited volume of soil, and the root is at the center of this cylinder (Claassen and Steingrobe 1999).
- For SSAND and PCATS, Roots are assumed to be parallel and distributed regularly throughout the soil volume (Baldwin 1973).

As a transient state model utilizing a numerical solution, NST 3.0 has been widely used to predict nutrient uptake by various crop species (Sadana and Claassen 2000; Satnam and Sadana 2002; Samal et al. 2003; Sadana et al. 2005; Pypers et al. 2006). However, we are not aware of any studies utilizing this model on a woody species. Transient state models utilizing a numerical solution are a well established approach to mechanistic nutrient uptake models (Tinker and Nye 2000). The Barber-Cushman model is a well-known and widely-used model in this category. NUTRIENT UPTAKE model and NST 1.0 are the personal computer version of the Barber-Cushman model (Claassen et al. 1986; Oates and Barber 1987). Since NST 3.0 is an improved version of NST 1.0, and all the data sets obtained from the literature for testing model predictive accuracy were developed for use with NUTRIENT UPTAKE model, the principles of NUTRIENT UPTAKE model and NST series are presented.

Nye and Spiers (1964) proposed the continuity equation that described the flux of nutrient in the soil to the root surface:

$$\frac{1}{r}\frac{\partial\left(rD\frac{\partial C_L}{\partial r}+\frac{v_0 r_0 C_L}{b}\right)}{\partial r}=\frac{\partial C_L}{\partial t} \qquad [1]$$

where r is the radial distance from the root, D is the diffusion coefficient, C_L is the nutrient concentration in the soil solution, v_0 is the water flux at the root surface, r_0 is the average root radius, b is the buffer power of the nutrient, and t is time. Nye and Marriot (1969) defined boundary conditions and solved this equation numerically.

Building on the work of Nye and Marriot (1969), Claassen and Barber (1976), and Cushman (1979a; 1979b), Barber and Cushman (1981) revised the boundary conditions of equation 1 to include inter-root competition for nutrients under both inner and outer boundary conditions:

(1) Inner boundary condition:

$$t > 0, r = r_0, F = Db\frac{\partial C_L}{\partial r}+v_0 C_L=\frac{\alpha C_L}{1+\alpha C_L/I_{max}}-E \qquad [2]$$

Where F is the flux of the nutrient, α is the root absorbing power, I_{max} is maximum net influx at high nutrient concentrations, E is the nutrient efflux of plant roots, and $(\frac{\alpha C_L}{1+\frac{\alpha C_L}{I_{max}}}-E)$ is a transformation of the Michaelis-Menten equation.

(2) Outer boundary condition:

If there is no inter-root competition,

$$t > 0, r = r_1, C_L = \text{constant} \qquad [3]$$

If there is inter-root competition,

$$t > 0, r = r_1, F = Db\frac{\partial C_L}{\partial r}+v_1 C_L=0 \qquad [4]$$

where v_1 is the water influx at the distance r_1.

The boundary conditions incorporated inter-root competition and Michaelis-Menten kinetics. When solved numerically, the enhanced mechanistic model evolved into the Barber-Cushman model. In 1983, Itoh and Barber made a change to the Barber-Cushman model so that it is able to simulate nutrient uptake by root hairs. In 1987, Oates and Barber published NUTRIENT UPTAKE model, which is a personal computer version of the Barber-Cushman model with the revision by Itoh and Barber (1983). In 1986 Claassen et al. published NST 1.0 model, which was based largely on the Barber-Cushman model. Later Claassen and his colleagues developed NST 2.0 and NST 3.0, which were not published in a journal (Claassen, N. Personal communication.

2009, 31 July). NST 3.0 incorporates the Freundlich isotherm into the model so that the buffer power (b) changes as the nutrient concentration in soil solution changes (Steingrobe et al. 2000).

Steady state models are another major standard category in mechanistic nutrient uptake modeling (Tinker and Nye 2000). Baldwin et al. (1973) and Nye and Tinker (1977) proposed the key equations. Based on their work, Smethurst and Comerford (1993b) developed a model, COMP8 (Competition model version 8), which was able to calculate nutrient uptake between two competing and contrasting root systems. SSAND is a revision and expansion of COMP8 by Comerford et al. (2006). Its main improvements lie in the functions of predicting nutrient uptake as influenced by mycorrhizae and simulation of fertilization effects (Comerford et al. 2006). Based on COMP8 and an earlier version of SSAND, another steady state model, PCATS was developed by Smethurst et al. (2004) to simulate nutrient uptake by a single species. In the following section, the principles of steady state models are briefly described, and the features of COMP8, SSAND and PCATS are introduced.

Based on the continuity equation of Nye and Spiers (1964), Baldwin et al. (1973) and Nye and Tinker (1977) proposed the key equations for the concentration profile around the root, as well as the average concentration for use in a steady state model.

$$\frac{C_{Lr}}{C_{L0}} = \frac{\alpha}{v_0} + \left[1 - \frac{\alpha}{v_0}\right] \left(\frac{r}{a}\right)^{-\left(\frac{r_0 v_0}{bD}\right)}$$

[5]

Where C_{Lr} is the nutrient concentration in soil solution at the distance r from the root, and C_{L0} is the nutrient concentration in soil solution at the root surface.

By representing the average concentration across the depletion zone with C_{av}, the relationship between C_{av} and C_{L0} can be obtained by

$$\frac{C_{av}}{C_{L0}} = \frac{\alpha}{v_0} + \left(1 - \frac{\alpha}{v_0}\right) \left(\frac{2}{2 - \frac{r_0 v_0}{bD}}\right) \frac{\left(\frac{r_1}{r_0}\right)^{\left(2 - \frac{r_0 v_0}{bD}\right)} - 1}{\left(\frac{r_1}{r_0}\right)^2 - 1}$$

[6]

Because the amount of nutrient uptake ΔU during the time period Δt is given by the equation:

$$\Delta U = 2\pi r_0 L_v \alpha C_{L0} \Delta t$$

[7]

ΔU can be calculated using equations 6 and 7:

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$$\Delta U = 2\pi r_0 L_v \alpha \Delta t \frac{C_{av} v_0}{\alpha + (v_0 - \alpha)(\frac{2}{2 - \frac{r_0 v_0}{bD}}) \frac{(\frac{r_1}{r_0})^{(2 - \frac{r_0 v_0}{bD})} - 1}{(\frac{r_1}{r_0})^2 - 1}} \qquad [8]$$

At time interval Δt_1, $C_{av1} = C_{Li}$. Therefore the new C_{av2} can be calculated from the uptake at time interval Δt_2, and C_{L02} can be calculated from C_{av2}. This approach allows any time period to be represented. Finally, the total amount of nutrient uptake can be obtained by summing ΔU at each time interval.

Another key equation which Smethurst and Comerford (1993b) based the development of COMP8 on is not discussed here because it is related to nutrient uptake by two competing roots. Smethurst and Comerford (1993b) also made the following improvements: (i) "a depletion zone that increased with time until it reached the no-transfer boundary, (ii) an adjustment in concentration to reflect newly encountered solutes in the depletion zone, (iii) a variable root absorbing power α (equation 9) to describe Michaelis-Menten uptake kinetics, and (iv) a routine to account for the competition between two root systems".

$$\alpha = \frac{I_{max}}{K_m + C_{L0} - C_{min}} \qquad [9]$$

Two verification studies with slash pine and weeds were conducted in the same year (Smethurst and Comerford 1993a; Smethurst et al. 1993). However, this model has had little use since 1993 because it was judged to be inadequate under some conditions possibly due to its inability to describe some components of the soil-root system such as root length development, changing soil moisture content, and nutrient input from mineralization (Smethurst and Comerford 1993b; Singh 2008).

Based on COMP8, SSAND included several new functions allowing simulation of nutrient uptake by roots under a variety of conditions such as mycorrhizal roots, fertilization, changing soil water content, nutrients from different soil horizons, and dynamic mineralization rates (Comerford et al. 2006). SSAND includes a sub-routine to calculate the nutrient demand for target plant growth, so that it can provide a recommendation on fertilization by comparing the predicted uptake and demand.

Similar to SSAND, PCATS is able to simulate nutrient uptake by mycorrhizae and uptake influenced by fertilization (Smethurst et al. 2004). However, it can only predict nutrient uptake

by one species. PCATS shares similar principles with COMP8 and SSAND, but further simplifies the calculation by running on a fixed daily time-step (Smethurst et al. 2004).

Usually transient state models with a numerical solution are considered to be more accurate than steady state models (Smethurst and Comerford 1993b; Yanai 1994). Numerical methods are those that "iteratively solve a system of simultaneous equations developed from approximations of the differential equation for solute transport" (Smethurst and Comerford 1993b). "The steady state approach assumes that the concentration profile around the root can be considered to be in a steady state" (Yanai 1994), which is usually attained after long times (Nye and Spiers 1964). Since natural phenomena are transient, the results obtained using this approach may not be as accurate as the transient state model.

The major advantage of a steady state model over a transient state model lies in "the independence of the mathematical solution to previous condition" during calculation (Yanai 1994) so that steady state models are able to respond to real-time changes in parameters. Transient state models using a numerical solution are also called "deterministic" models (Claassen and Steingrobe 1999) because the simulation does not accept time-varying input (Yanai 1994). For example, soil moisture is not allowed to change during the calculation, though it is unrealistic to think that soil moisture would remain constant in the field.

Data Used for Comparison of NST 3.0, SSAND, and PCATS

Data were taken from three studies conducted by Kelly et al. (1992), Kelly et al. (2001), and Kelly and Ericsson (2003). The study by Kelly et al. (1992) verified the use of the NUTRIENT UPTAKE model on the simulation of phosphorus, potassium, and magnesium uptake by 1-0 loblolly pine seedlings growing in a modified A horizon soil (Lily series) for 180 days. Two sets of data were taken from this study.

The study by Kelly et al. (2001) largely focused on the influence of environmental factors and plant growth on parameter values used by NUTRIENT UPTAKE model. They measured the model parameters of 1-year-old black cherry, northern red oak, and red maple seedlings in pots with A horizon soils from two forest sites in the Great Smoky Mountains National Park in Tennessee. Two sets of data on red maple grown in the Cove Mountain soil were taken from this study. The study of phosphorus uptake was not included because of the authors did not detect any phosphorus in the soil solution obtained.

Uptake of nitrate, phosphorus, and potassium by hybrid poplar cuttings was simulated for either 30 or 105 days by Kelly and Ericsson (2003) using the NUTRIENT UPTAKE model. A steady state technique to assure maximal relative growth rate at three fertilizer additions (different amounts of 17-6-12 fertilizer addition equivalent to 0, 75, and 150 kg ha^{-1} of nitrogen) were included in the experiment. Nine data sets were taken from this study.

Data transformation

The inputs for NST 3.0, SSAND, and PCATS differ in some ways from those used for NUTRIENT UPTAKE model. SSAND provides the user great flexibility to define various scenarios. For example, the user of SSAND and PCATS can define more than one soil horizon that the plants explore and can specify different parameters in each horizon. The number of parameters also depends on the way the user collects data. Because all data sets obtained from the studies of Kelly et al. (1992), Kelly et al. (2001), and Kelly and Ericsson (2003) were developed for use with NUTRIENT UPTAKE model, data transformations were required.

Unlike NUTRIENT UPTAKE model which uses a fixed value of buffer power (b), all three models allow users to input parameters to define a sorption equation so that b can be calculated as the nutrient concentration in the soil solution changes as plant uptake occurs. This function is slightly different among the models. NST 3.0 and PCATS allow the user to define only a Freundlich equation for the absorption isotherm. SSAND uses different adsorption and desorption isotherms, and allows the user to choose either a Freundlich or Langmuir equation to fit these sorption isotherms. Because the studies of Kelly et al. (1992), Kelly et al. (2001), and Kelly and Ericsson (2003) followed the methodology of Barber (1995) and the buffer power of the soil is the nutrient concentration per unit soil volume (C) divided by the concentration in soil solution (C_L):

$$b = C/C_L \qquad [10]$$

The isotherm equations for the three models were set as

$$C = b * C_L \qquad [11]$$

Like NUTRIENT UPTAKE model, NST 3.0 requires the user to input a fixed value for the tortuosity factor (f). SSAND provides several functions that the user can choose to define a formula for calculating f with volumetric soil moisture θ. PCATS works similarly to SSAND in this aspect, except that it provides only one slightly different function. The formulas used in our

simulation were first proposed by Kovar and Barber (1990). That is, if the soil is > 75% sand and $\theta < 0.15$ m^{3}m^{-3} at field capacity,

$$f = 0.25\theta \qquad [12]$$

Otherwise

$$f = 1.58\theta - 0.172 \qquad [13]$$

When an absorption isotherm is introduced into the model, buffer power (b) is no longer fixed and changes as C_{Li} changes. The effective diffusion coefficient (D_e) can also vary during simulation because it is related to b. Since NST 3.0, SSAND, and PCATS require the user to define sorption isotherms, D_e is not an input parameter in these models and is replaced by volumetric soil moisture (θ) and the diffusion coefficient in water of the nutrient (D_L).

NST 3.0 uses the half distance between root axes (r_1) at the end of the experiment rather than the average r_1 over the experimental period. SSAND and PCATS do not require the user to input r_1. Instead, PCATS requires the input of root length density on a daily basis. SSAND can calculate nutrient uptake by assuming no root growth occurred with a specified root length density, or it can use an Excel file to input daily root length density using the same format as PCATS.

Both SSAND and PCATS require user input on soil bulk density and soil volume. PCATS further requires the user to define the percentage of soil volume that is occupied by roots. Because of the lack of information in the literature, the soil volume was assigned as the pot size in the SSAND simulation, and the percentage of the soil volume that was occupied by roots was assumed to be 1. The same assumptions were used in the PCATS simulation in order to keep the input the same as SSAND.

Since PCATS is designed specifically for predicting phosphorus uptake by plants, its simulated results (U_P) are calculated as μmols of phosphorus uptake during the time period. Therefore, the actual simulated results (U) are transformed with the following formula:

$$U = U_P * \frac{atomic\ weight\ of\ phosphorus}{atomic\ weight\ of\ the\ nutrient} \qquad [14]$$

The values for the parameters used in each model are listed in Tables 6 and 7, values that are not listed are discussed below. For NST 3.0, three parameters (a, b, and c) are used to define the sorption isotherm using the simplified isotherm equation 11, b equals to the buffer power, while

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Table 6. Parameter values for loblolly pine and red maple based on observations reported by Kelly et al. (1992) and Kelly et al. (2001) used for NST 3.0, SSAND and PCATS simulations.

Parameters	Units	Loblolly pine (Kelly et al. (1992))		Red maple (Kelly et al. (2001))	
		K	P	NO_3-N	K
D_L [†‡§]	$cm^2\ s^{-1}$	1.98E-05	8.90E-06	1.90E-05	1.98E-05
θ [†‡]	unitless	0.062		0.44	
v_0 (or LI rate) [†‡]	$cm\ s^{-1}$	5.66E-07		5.17E-06	
C_{li} [†‡]	$\mu mol\ ml^{-1}$	0.27	0.19	0.51	0.13
b [†‡]	unitless	10.55	5.84	1.35	7.02
I_{max} [†‡]	$\mu mol\ cm^{-2}\ s^{-1}$	1.40E-06	2.68E-07	3.09E-05	3.80E-06
K_m [†‡]	$\mu mol\ ml^{-1}$	0.03	0.016	0.32	10.46
C_{min} [†‡]	$\mu mol\ ml^{-1}$	0.001	0.0006	0.001	0.003
r_0 [†‡]	cm	0.035		0.044	
r_1 [†]	cm	1.65		0.903	1.186
L_0 [†]	cm	285		1696	
k [†]	$cm\ day^{-1}$	14		41.04	
simulated time [†‡]	day	180		30	176
Soil volume [‡]	cm^3	24000		7500	
Bulk density [‡]	$g\ cm^{-3}$	0.75		0.74	

† parameters used by NST 3.0
‡ parameters used by SSAND and PCATS
§ The values of D_L for nitrate and potassium were taken from Parsons (1959), and that of phosphorus from Edwards and Huffman (1959).

Table 7. Parameter values for hybrid poplar based on observations reported by Kelly and Ericsson (2003) used for NST 3.0, SSAND and PCATS simulations.

Parameters	Units	No fertilizer addition			75kg ha^{-1} of fertilizer addition			150kg ha^{-1} of fertilizer addition		
		NO$_3$-N	P	K	NO$_3$-N	P	K	NO$_3$-N	P	K
D_L[†‡§]	cm^2 s^{-1}	1.90E-05	8.90E-06	1.98E-05	1.90E-05	8.90E-06	1.98E-05	1.90E-05	8.90E-06	1.98E-05
θ[†‡]	unitless		0.27			0.28			0.28	
v_0(or LI rate)[†‡]	cm s^{-1}		7.46E-07			7.46E-07			7.46E-07	
C_{Li}[†‡]	µmol ml^{-1}	0.0761	0.0021	0.0963	1.52	0.0086	0.217	2.31	0.0388	0.519
b[†‡]	unitless	1.14	180.5	5.095	1.98	52.23	2.62	1.42	15.41	1.4
I_{max}[†‡]	µmol cm^{-2} s^{-1}	2.85E-05	1.51E-06	1.76E-05	2.85E-05	1.51E-06	1.76E-05	2.85E-05	1.51E-06	1.76E-05
K_m[†‡]	µmol ml^{-1}	0.712	0.00087	0.0269	0.712	0.00087	0.0269	0.712	0.00087	0.0269
C_{min}[†‡]	µmol ml^{-1}	0.001	0.001	0.003	0.001	0.001	0.003	0.001	0.001	0.003
r_0[†‡]	cm		0.02			0.02			0.02	
r_1[†]	cm		0.42			0.26			0.26	
L_0[†]	cm		1094			779			976	
k[†]	cm day^{-1}		29.98			97.63			94.18	
Simulation time[†‡]	day		105			105			105	
Soil volume[‡]	cm^3		2357			2357			2357	
Bulk density[‡]	g cm^{-3}		1.4			1.41			1.4	

† parameters used by NST 3.0

‡ parameters used by SSAND and PCATS

§ The values of D_L for nitrate and potassium were taken from Parsons (1959), and that of phosphorus from Edwards and Huffman (1959).

a and c were set as 1 and 0 for every run. The number of compartments used for numerical calculations was set to 40 for each run. For SSAND, the adsorption and desorption isotherm were assumed to be the same. The Freundlich equation was chosen as the adsorption and desorption type, and the same simplified isotherm equation was used. Equation 12 or 13 was used to define the impedance factor (f), depending on volumetric soil moisture and soil texture. For PCATS, the parameters for the sorption isotherm were set the same as in the other two models. Because the unique function provided by PCATS for calculating impedance factor is different, the value of the parameter of the impedance factor equation was adjusted so that the calculated impedance factors of PCATS were the same as the others. For both SSAND and PCATS, which require the user to define root length density day by day, the root length density for the first day was calculated by dividing initial root length by soil volume. For subsequent days the root length density increases linearly with the step value equal to the root growth rate (cm day^{-1}) divided by soil volume.

Methods of sensitivity analysis

The traditional or one dimensional sensitivity analysis was first used to by Silberbush and Barber (1983) to show the influence of different parameters on model simulations. It was accomplished by changing a single model input parameter while keeping the others constant (Silberbush and Barber 1983). By plotting the change ratio of the parameters compared to their original values on the horizontal axis, and the predicted uptake to the original prediction on the vertical axis, it is possible to evaluate the importance of each parameter by the slope of the lines on the graph. This procedure has been largely followed in subsequent analyses.

Following the methodology developed by Silberbush and Barber (1983), a one dimensional sensitivity analysis was conducted using the data of Kelly et al. (1992) for potassium uptake by loblolly pine seedlings. Each of the parameters was changed by a factor of 0.5, 0.75, 1.25, 1.5, or 2 times the original level while the remaining parameters were held constant. Those parameters that are dependent on other parameters were not included in the sensitivity analysis. Claassen and Steingrobe (1999) suggested doing sensitivity analysis with the C_{Li} and b combined. Since an isotherm equation for the Kelly et al. (1992) study was not available, and the simplified relationship between C_L and b (equation 11) is not theoretically accurate, the sensitivity analysis

was done using individual C_{Li} and b. Therefore, ten parameters were evaluated in the one dimensional sensitivity analysis of each model.

Yanai (1994) proposed the concept of multiple dimensional sensitivity analysis and conducted several two dimensional sensitivity analyses using the steady state model developed by Baldwin et al. (1973) and Nye and Tinker (1977). Williams and Yanai (1996) conducted a multiple dimensional sensitivity analysis using a simplified steady state model across a range of values described in the literature. By changing each parameter at 4 levels, 16,384 parameter datasets were created. Using ANOVA, they identified the average nutrient concentration in the soil solution (C_{av}), maximal rate of nutrient uptake (I_{max}), root radius (r_0), and the effective diffusion coefficient (D_e), to be the most important parameters that control uptake per unit length of root (Williams and Yanai 1996). Root radius r_0 becomes less important when uptake rates are expressed on a surface basis (Williams and Yanai 1996). They then represented selected parameters at 5 levels and plotted the response surface using a series of graphs. The response surfaces developed using this method indicated clear relationships between the selected parameters.

Because SSAND and PCATS share similar principles in modeling and response patterns in the one dimensional sensitivity analysis, only SSAND and NST 3.0 were compared using the multiple dimensional sensitivity analysis. Results obtained from the one dimensional sensitivity analysis indicated that C_{Li}, θ, k, r_0, and v_0 were the most influential parameters. Williams and Yanai (1996) found that C_{Li} (or C_{av}), D_e, and I_{max} were the most influential parameters in their multiple dimensional sensitivity analysis with a simplified steady state model. Therefore, C_{Li} and θ were chosen for further evaluation in the current study because of their prominent effects in the one dimensional sensitivity analysis. Williams and Yanai (1996) did not take root growth (k) or other root morphological parameters into account. But studies on modeling of nutrient uptake by woody species (Van Rees et al. 1990; Smethurst and Comerford 1993b; Comerford et al. 2006; Singh 2008), including our own one dimensional sensitivity analysis, showed that k was an important parameter for nutrient uptake by woody species. Because all three models simulate nutrient uptake on a surface area basis, plus the fact that the range of average root radius (r_0) for a species is narrow, r_0 was not included in the current multiple dimensional sensitivity analysis. Although v_0 is among the most influential parameters in our one dimensional sensitivity analysis,

it is not included in the multiple dimensional sensitivity analysis because the uptake of potassium is mainly by diffusion (Barber 1995), the importance of v_0, a major parameter for mass flow, is not as important. While Williams and Yanai (1996) defined I_{max} as one of the most influential parameters, the range of I_{max} for loblolly and slash pine was narrow, from 1.4E-6 µmol cm^{-2} s^{-1} (Kelly et al. 1992) to 3.65E-6 µmol cm^{-2} s^{-1} (Kelly et al. 1995). Although its actual range may be much wider, it is hard to artificially define a range for this parameter. Therefore, I_{max} was excluded in the multiple dimensional sensitivity analysis. As a result, C_{Li}, θ, and k were selected as the three parameters for evaluating the multiple dimensional sensitivity analysis.

The ranges of values for these parameters were taken from the literature. Because the number of studies on measuring model parameters of loblolly pine is limited, data on slash pine were included to build reasonably representative ranges of the three parameters. The values and sources of the data are listed in Tables 8, 9, and 10. Based on these values, the range for volumetric soil moisture (θ) was 0.06 to 0.4, the range for nutrient concentration in the soil solution (C_{Li}) was 0.028 µmol ml^{-1} to 8.54 µmol ml^{-1}, and the range for root growth rate (k) was 1 cm day^{-1} to 39.3 cm day^{-1}.

Each of the three parameters was varied linearly at five levels across the range, giving 125 "observations" in the data set for each of the two models. Using the obtained results, two graphical representations similar to those of Williams and Yanai (1996) were developed to show the relationship of the parameters and their influences on the simulations.

Results and Discussion

Calculation of uptake using data taken from the literature

Most model simulations underpredict nutrient uptake by 2% to 100% (Table 11). Five simulations of potassium uptake were run with NST 3.0, SSAND, and PCATS (Figure 1). For four out of the five simulations NST 3.0 and PCATS predicted 8 to 54% of the observed uptake. The prediction of uptake by hybrid poplar under the no fertilizer treatment was 125% and 83% for NST 3.0 and PCATS, respectively. SSAND predicted 7 to 50% of the observed uptake in all simulations.

Table 8. Literature values for soil moisture (θ) taken from field, nursery, and greenhouse studies of loblolly and slash pine.

Species and study type	θ	Data source
Slash pine, field study	0.24-0.3	(Van Rees et al. 1990)
Slash pine, nursery study	0.12-0.17	(Van Rees et al. 1990)
Slash pine, field study, soil depth measured: 0-10 cm	0.1-0.3	(Smethurst et al. 1993)
Slash pine, field study, soil depth measured: 10-26 cm	0.1-0.4	(Smethurst et al. 1993)
Slash pine, field study, soil depth measured: 26-50 cm	0.2-0.4	(Smethurst et al. 1993)
Slash pine, field study, soil depth measured: 50-70 cm	0.3-0.4	(Smethurst et al. 1993)
Slash pine, field study	0.17-0.23	(Smethurst and Comerford 1993a)
Loblolly pine, field study	0.15	(Comerford et al. 2006)
Loblolly pine, greenhouse study	0.062	(Kelly et al. 1992)

Table 9. Literature values for potassium concentration in soil solution (C_{Li}) taken from field, nursery, and greenhouse studies of loblolly and slash pine.

Species	C_{Li} (μmol ml^{-1})	Data source
Loblolly pine	0.27	(Kelly et al. 1992)
Loblolly pine	0.99-8.54	(Kelly et al. 1995)
Slash pine	0.035-0.203	(Van Rees et al. 1990)
Slash pine	0.0382-0.338	(Smethurst and Comerford 1993a)
Slash pine	0-0.46	(Smethurst et al. 1993)

Table 10. Literature values of root growth rate (k) taken from field, nursery, and greenhouse studies of loblolly and slash pine.

Species	k (cm s^{-1})	Data source
Slash pine	0.000012-0.000184	(Van Rees et al. 1990)
Slash pine	0.000064-0.000455	(Van Rees and Comerford 1990)
Loblolly pine	0.00004-0.00013	(Kelly et al. 1995)
Loblolly pine	0.000162	(Kelly et al. 1992)

Four simulations of nitrate uptake were run with the three models (Figure 2). The percentages for the model predictions divided by the observed uptake for each model is relatively constant. NST 3.0 and SSAND underpredicted nitrate uptake by about 50%. PCATS predicted nitrate uptake by hybrid poplar in the three fertilizer treatments at 98%, 98%, and 85% of the observed. Red maple uptake of nitrate as described by PCATS was 61% of the observed uptake.

Four simulations of phosphorus uptake were run with each model (Figure 3). SSAND and PCATS responded very similar and predicted 20% of the observed uptake in the loblolly pine study, and less than 1% of the observed uptake in the hybrid poplar study. On the other hand, NST 3.0 predicted 61% of the observed phosphorus uptake for the loblolly pine study. The prediction by NST 3.0 of phosphorus uptake by hybrid poplar improved as the fertilizer addition increased and the best prediction (110% of the observed uptake) occurred with the highest fertilizer addition.

NST 3.0, SSAND, and PCATS produced diverse results using the same data (Table 11). For nitrate uptake simulation, PCATS had the closest estimates to the observed uptake, while the performance of NST 3.0 and SSAND are similar. For phosphorus uptake simulation, the performance of NST 3.0 was greatly improved when applied to situations with fertilization, and this was in accordance with the observation of Van Rees et al. (1990) that the Barber-Cushman model worked well in the tree nursery when fertilizers were added. Both SSAND and PCATS predicted phosphorus uptake of hybrid poplar to be less than 1 µmol, while the observed uptake ranges from 52 µmol to more than 1000 µmol. No obvious pattern was observed in the simulations of potassium uptake by the three models.

In an earlier model comparison study, Van Rees et al. (1990) evaluated potassium uptake by slash pine seedlings growing in a greenhouse, a tree nursery, and the field using the Barber-Cushman model and the Baldwin-Nye-Tinker model. The authors found that the simulated uptake of the latter model was 5% higher than the former in all of their studies. As successors of the Barber-Cushman and Baldwin-Nye-Tinker models, NST 3.0, SSAND, and PCATS produced simulated results with a much lower level of agreement.

Although NST 3.0 and PCATS performed relatively well with some runs, there was not a general pattern in the performance of the models in predicting major nutrient uptake in the three studies of coniferous and deciduous species taken from the literature. For example, potassium is

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Table 11. Observed uptake of NO$_3$-N, P, and K compared to simulated uptake as predicted by NST 3.0, SSAND, and PCATS using data from Kelly et al. (1992), Kelly et al. (2001), and Kelly and Ericsson (2003). The percentages represent the degree of correspondence between the simulated and observed uptake value.

| Experiments	Nutrient	Observed uptake (µmol)	Simulated uptake (µmol)					
			NST 3.0		SSAND		PCATS	
Loblolly pine (simulation time: 180 days)								
	K	6663	1020	15%	466	7%	510	8%
	P	1332	596	45%	265	20%	270	20%
Red maple (simulation time for N: 30 days; for K: 176 days)								
	NO$_3$-N	8810	4160	47%	4277	49%	5370	61%
	K	1890	983	52%	950	50%	1016	54%
Hybrid poplar (simulation time: 105 days)								
0 kg ha^{-1} of fertilizer addition	NO$_3$-N	346	167	48%	216	62%	309	89%
	P	170	52.3	31%	0	0%	0.0004	0%
	K	719	900	125%	158	22%	600	83%
75 kg ha^{-1} of fertilizer addition	NO$_3$-N	11000	6000	55%	5411	49%	10814	98%
	P	581	489	84%	0.05	0%	0.001	0%
	K	4302	1090	25%	662	15%	1562	36%
150 kg ha^{-1} of fertilizer addition	NO$_3$-N	14429	6590	46%	6701	46%	12235	85%
	P	940	1030	110%	1.01	0%	0.0006	0%
	K	5624	1380	25%	1364	24%	2467	44%
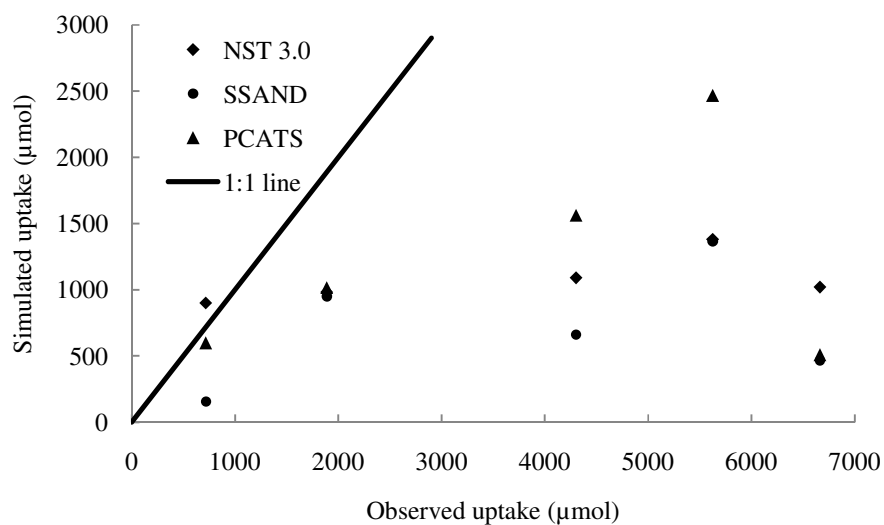
Figure 1. Comparison of predicted potassium uptake by the NST 3.0, SSAND, and PCATS models and observed potassium uptake using data from the studies by Kelly et al. (1992), Kelly et al. (2001), and Kelly and Ericsson (2003).
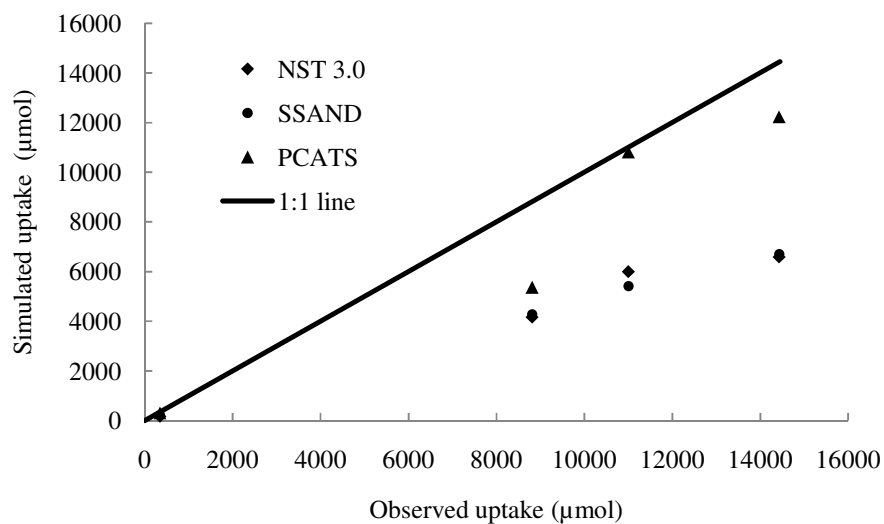

Figure 2. Comparison of predicted nitrate uptake by the NST 3.0, SSAND, and PCATS models and observed nitrate uptake using data from the studies by Kelly et al. (1992), Kelly et al. (2001), and Kelly and Ericsson (2003).
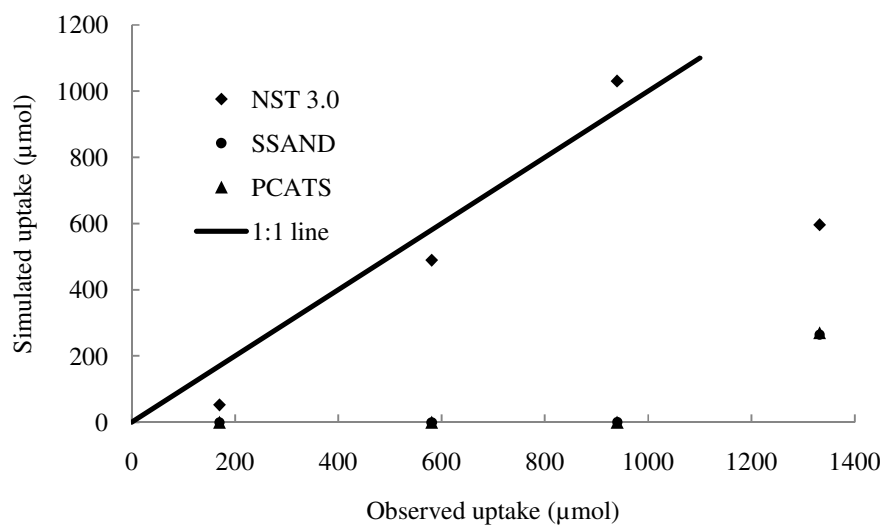
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Figure 3. Comparison of predicted phosphorus uptake by the NST 3.0, SSAND, and PCATS models and observed phosphorus uptake using data from the studies by Kelly et al. (1992), Kelly et al. (2001), and Kelly and Ericsson (2003).

considered to be easier to model than other major nutrients because the components of the potassium cycle in the soil are less complex than nitrogen and its reactions with soil particles or root surfaces are simpler than phosphorus (Tinker and Nye 2000). But the ranges of the percentages of the predicted against observed values by the three models (Table 11) were wide. The fact that the best simulations of NST 3.0 and SSAND occurred in the hybrid poplar study under the no fertilizer treatment contradicts the opinion that mechanistic nutrient models work better under the conditions when soil supply of nutrients is abundant (Van Rees et al. 1990).

Therefore, our study indicates that the prediction of nutrient uptake by NST 3.0 SSAND, and PCATS using the same dataset can be diverse, but it is unclear that why such differences occurred. The lack of estimates on mycorrhizal uptake of nutrients may be an important reason that most simulations underestimated nutrient uptake. Further studies producing representative datasets that both reflect soil and plant characteristics of woody species scenarios are required.

Sensitivity analysis

One dimensional sensitivity analysis

SSAND and PCATS produce similar patterns in the one dimensional sensitivity analysis (Figures 4 and 5). Listed in order of their importance, the most influential parameters were: $\theta > C_{Li} > k > v_0 > r_0$. The analysis also shows that both I_{max} and C_{min} have similar negative influences on uptake estimates from the two models. For example, increasing I_{max} by a factor of 2 decreases the predicted uptake by 35% and 26% for SSAND and PCATS, respectively. The change ratios for θ, C_{Li}, v_0, K_m, C_{min}, and I_{max} in SSAND indicate a greater influence on simulated results than those of PCATS. The influence of k, L_0, and b on the simulated results of the two models was almost the same. Only the influence of r_0 is less in SSAND than in PCATS (Figures 4 and 5).

The one dimensional sensitivity analysis response of NST 3.0 is different from those of SSAND and PCATS (Figure 6). If listed in the order of significance, the most influential parameters in this sensitivity analysis of NST 3.0 were $C_{Li} > r_0 = k > \theta > v_0$. Note that the influence of θ is not as prominent in NST 3.0 as it is in SSAND and PCATS. The uptake kinetics parameters (I_{max}, K_m, and C_{min}) have no influence on NST 3.0 simulations, while for SSAND and PCATS, I_{max} and C_{min} had equally significant negative influences and K_m had a slight positive influence. Finally, NST 3.0 is the least sensitive model of the three to changes in parameter values. For example, if the value of a parameter is increased by a factor of 2, the subsequent

change ratio of results for NST 3.0 ranges from 1 to 2, while that of SSAND ranges from 0.65 to 2.55, and PCATS ranges from 0.74 to 2.42.

Williams and Yanai (1996) explained the interactions of soil and plant factors in controlling nutrient uptake by "distinguishing whether the rate of nutrient uptake is more limited by the potential rate of nutrient delivery to the root, which depends on soil properties, or by the potential rate of nutrient uptake into the root, which depends on root physiology". In this one dimensional sensitivity analysis of NST 3.0, SSAND, and PCATS for potassium uptake by loblolly pine seedlings, the uptake kinetics parameters either have little or negative influences, and nutrient concentration in soil solution and volumetric soil moisture were among the most influential parameters. Therefore, it appears that potassium uptake by loblolly pine seedlings taken from Kelly et al. (1992) was limited mainly by soil nutrient supply.

The influence of volumetric soil moisture, as represented by θ, is a relatively new parameter in the model sensitivity analysis. It is included in NST 3.0, SSAND, and PCATS, but was not used in the NUTRIENT UTPAKE model. Most nutrient uptake studies using SSAND or NST 3.0 exclude θ in the sensitivity analysis (Sadana and Claassen 1999; Sadana and Claassen 2000; Gill et al. 2005; Comerford et al. 2006). There are two studies where θ was included in the sensitivity analysis. These authors found that θ was among the most influential parameters in both studies (Smethurst and Comerford 1993b; Singh and Sadana 2002). Williams and Yanai (1996) identified C_{av}, I_{max}, and D_e as the most influential parameters in their multiple dimensional sensitivity analysis on a root surface area basis with a simplified steady state model. Because $D_e = f\theta D_L/b$, the value of D_L is relatively fixed, and f is a function of θ, the parameters replacing D_e in NST 3.0, SSAND, and PCATS include θ and b. From the equation we also notice that D_e is quadratically related to θ. And this may explain why θ is more influential than b in the sensitivity analysis.

The negative influence of I_{max} on simulated results in the one dimensional sensitivity analysis of SSAND and PCATS is surprising. No similar reports have been found. Three studies on nutrient uptake by woody species with a steady state model are available. Smethurst and Comerford (1993b) and Comerford et al. (2006) found no negative influence of I_{max} in COMP8 and SSAND simulations. Singh (2008) reported on the use of SSAND to simulate ammonium, nitrate, phosphorus, and potassium uptake by hybrid poplar growing on two soils. The study used
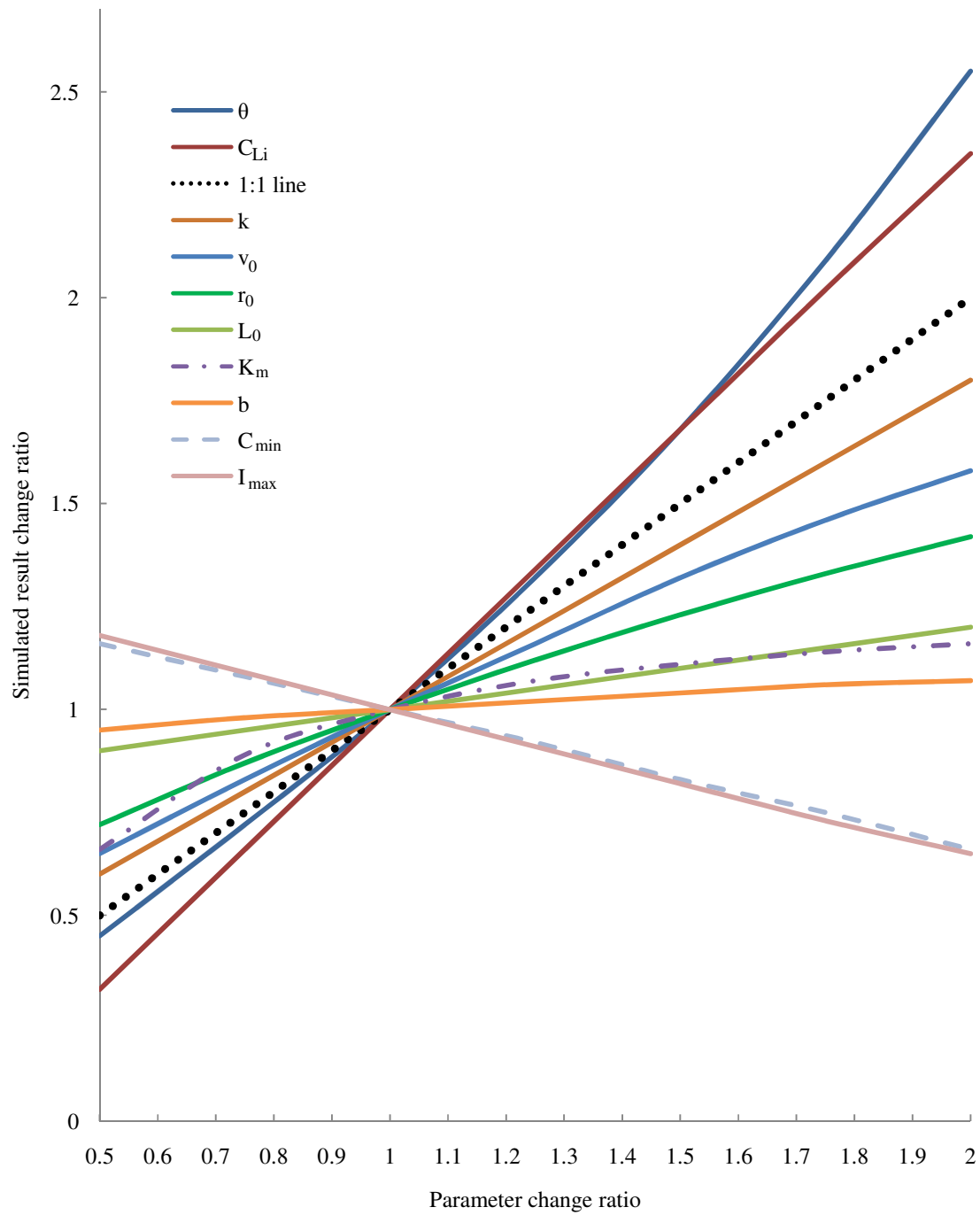
Figure 4. One dimensional sensitivity analysis using SSAND with potassium uptake data for loblolly pine seedlings from Kelly et al. (1992) and the diffusion coefficient of potassium in water at 25 ºC taken from the Parsons (1959).
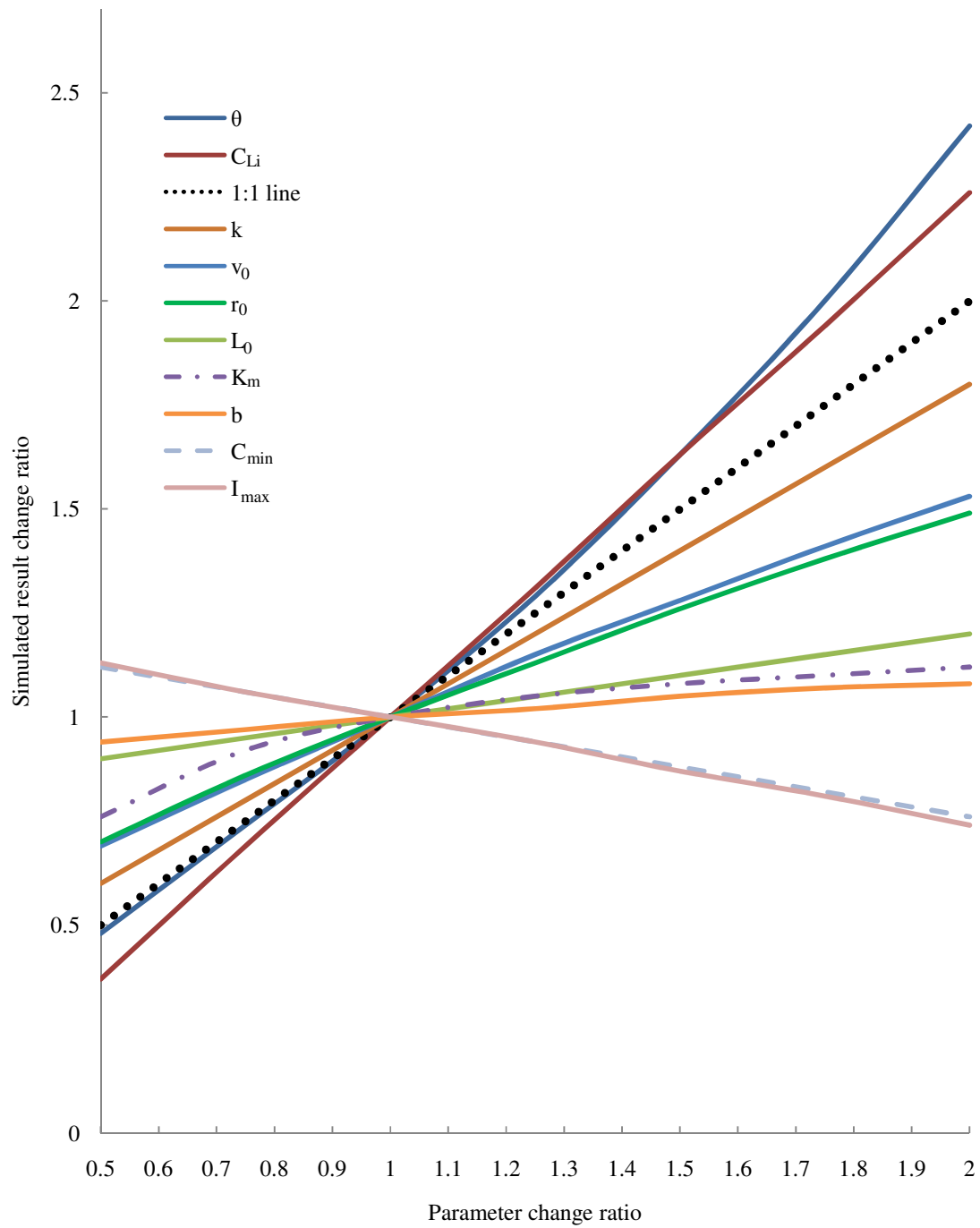
Figure 5. One dimensional sensitivity analysis using PCATS with potassium uptake data for loblolly pine seedlings from Kelly et al. (1992) and the diffusion coefficient of potassium in water at 25 ºC taken from the Parsons (1959).
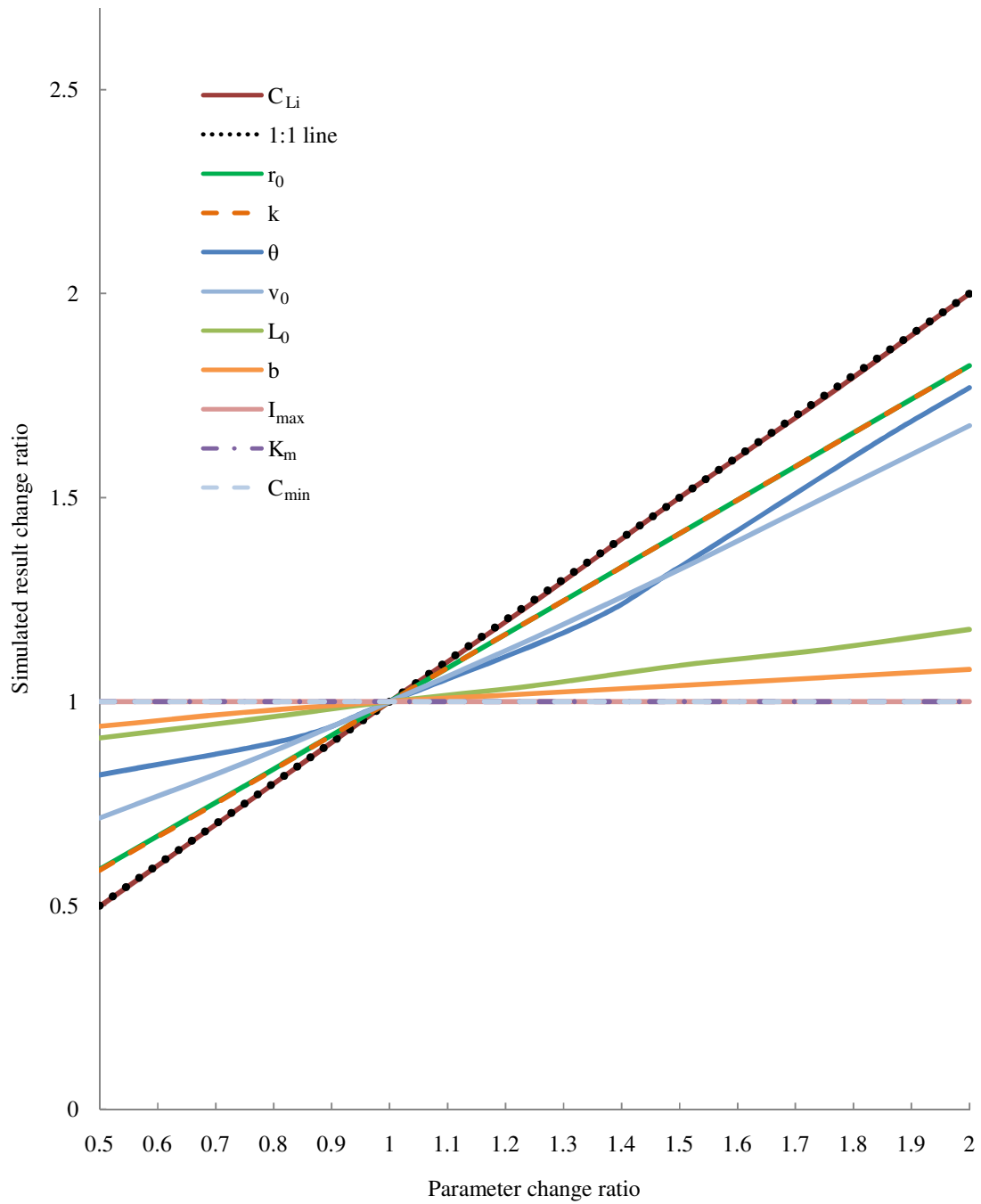
Figure 6. One dimensional sensitivity analysis using NST 3.0 with potassium uptake data for loblolly pine seedlings from Kelly et al. (1992) and the diffusion coefficient of potassium in water at 25 ºC taken from the Parsons (1959).

2 harvests and 16 simulations. The slope of the line representing I_{max} in the sensitivity analysis of ammonium uptake at the second harvest on both soils, and of potassium uptake in the second harvest on one of the soils, were slightly negative. Unfortunately the author did not discuss this phenomenon and summarized parameter values regardless of soil type and harvests such that it is difficult to explore further with their data. Because the negative influence of I_{max} in the Singh (2008) study was found at the second harvest when soil nutrients were depleted, and the most influential parameters in the one dimensional sensitivity analysis were related to soil properties, we suspect that the uptake process was limited by soil supply of nutrients and it seems that the negative influence of I_{max} is related to a limited supply of nutrients by the soil.

To explore this phenomenon, we examined the effects of I_{max} on uptake simulation with artificial datasets. In these data sets, root growth rate were set as 39.3 cm day^{-1}, and volumetric soil moisture was set as 0.4 (see multiple dimensional sensitivity analysis), so that they are not limiting soil supply or plant uptake process. The value of C_{Li} was varied linearly at 5 levels, ranging from 0.028 to 8.54 µmol ml^{-1}. In this case, we assume the nutrient supply of the soil increases as C_{Li} increases. I_{max} values for potassium uptake by loblolly and slash pine taken from the literature (Van Rees et al. 1990; Kelly et al. 1992; Kelly et al. 1995) range from 1.4E-6 to 3.65E-6 µmol cm^{-2} s^{-1}. Because the actual I_{max} may be very different, five levels of I_{max}, 1.4E-7, 1.4E-6, 3.65E-6, 1.4E-5, and 1.4E-4 µmol cm^{-2} s^{-1}, were used in order to get a comprehensive understanding of model behavior.

The results of this analysis are shown in Figure 7. When C_{Li} was equal to 0.028 µmol ml^{-1}, uptake simulated by SSAND was significantly lower than that of NST 3.0. The prediction by SSAND increased as I_{max} increased from 1.4E-7 to 1.4E-6 µmol cm^{-2} s^{-1}, and then dropped as I_{max} increased further, while the prediction of NST 3.0 increased as I_{max} increased. Thus the pattern of simulated uptake by SSAND as I_{max} increased shows a bell shape, compared to an exponential shaped curve by NST 3.0. When C_{Li} was increased to 2.156 µmol ml^{-1}, both models had similar predictions and patterns before I_{max} reached 1.4E-5 µmol cm^{-2} s^{-1}. The prediction of NST 3.0 still increased as I_{max} increased, while the prediction by SSAND dropped when I_{max} increased from 1.4E-5 to 1.4E-4 µmol cm^{-2} s^{-1}. The patterns of model behavior under different levels of C_{Li} higher than 4.284 µmol ml^{-1} were similar. The predictions of both models were close and increased as I_{max} increased when I_{max} ranged from 1.4E-7 to 1.4E-5 µmol cm^{-2} s^{-1}. The
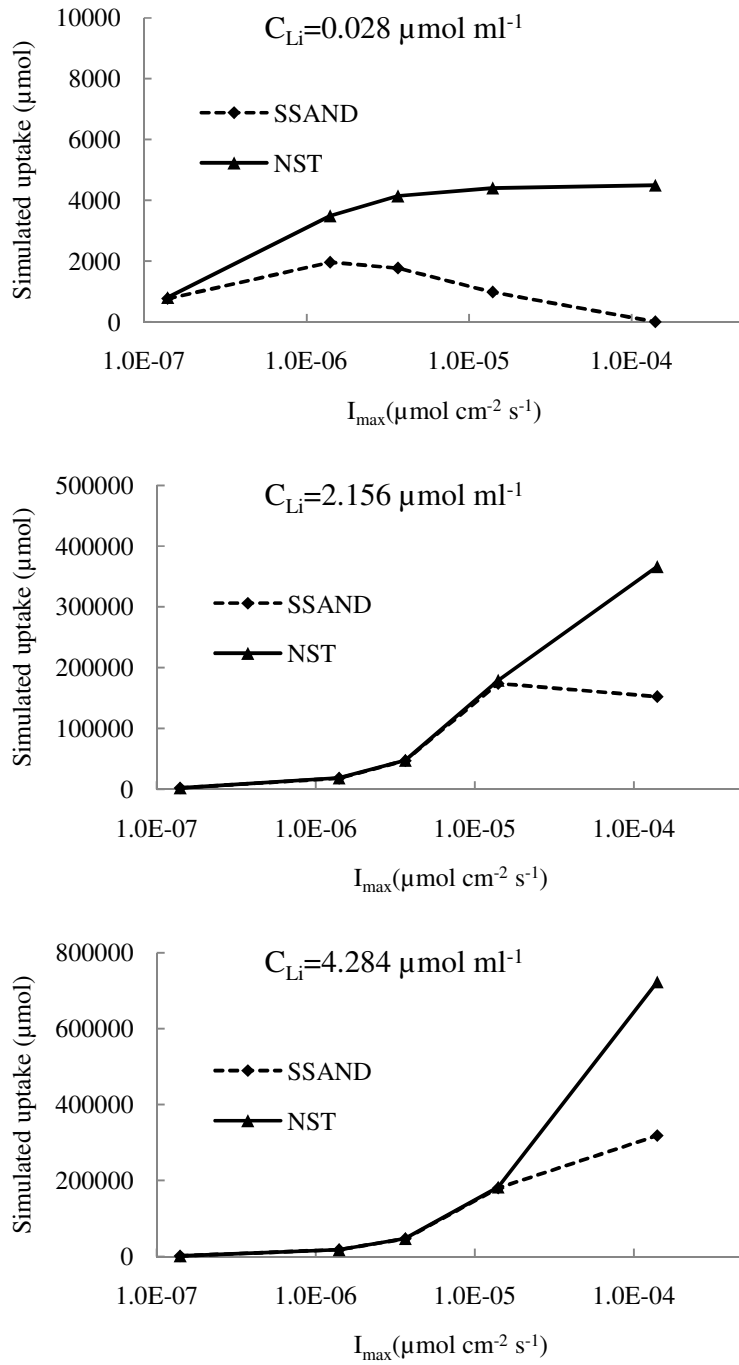
Figure 7. Simulated potassium uptake by SSAND and NST 3.0 at five levels of I_{max} and three levels of C_{Li}. For these simulations root growth rate and volumetric soil moisture have been set to 39.3 cm day^{-1} and 0.4 respectively. Other parameter values remained as listed in Table 6 for loblolly pine (Kelly et al. 1992).

prediction of SSAND was lower than that of NST 3.0 when I_{max} was equal to 1.4E-4 µmol cm^{-2} s^{-1}. Therefore, the behavior of SSAND is influenced by levels of C_{Li}, which indicates the ability of the soil to supply nutrients in our assumption. Our suspicion that the negative influence of I_{max} on SSAND simulation relates to the low nutrient supply by the soil is supported.

Previous studies with transient state models with a numerical solution have not reported a negative influence of I_{max} in the sensitivity analysis (Van Rees et al. 1990; Teo et al. 1992; Sadana and Claassen 1999; Sadana and Claassen 2000; Sterckeman et al. 2004; Gill et al. 2005; Comerford et al. 2006). In addition, the graphical representation in the multiple dimensional sensitivity analysis of a simplified steady state model by Williams and Yanai (1996) did not show a negative response in simulated uptake when I_{max} increased. According to the Michaelis-Menten uptake kinetics equation, nutrient influx into roots is positively related to I_{max}. Because nutrient uptake by plants is the accumulation of influx over time and root surface area, it is illogical to think that increased I_{max} would lead to a decrease in uptake. Therefore, we examined the key equation of the steady state model.

If A is used to represent $2\pi r_0 L_v \Delta t$, and B for $(\frac{2}{2-\frac{r_0 v_0}{bD}}) \frac{(\frac{r_1}{r_0})^{(2-\frac{r_0 v_0}{bD})}-1}{(\frac{r_1}{r_0})^2-1}$, then the key equation 8 of the steady state model can be rewritten as

$$\Delta U = A\alpha \frac{C_{av} v_0}{\alpha + B(v_0 - \alpha)} \tag{15}$$

If D is used to represent $\frac{1}{K_m + C_{L0} - C_{min}}$, then equation 9 can be rewritten as

$$\alpha = D * I_{max} \tag{16}$$

Then

$$\Delta U = \frac{A C_{av} v_0 I_{max}}{\frac{B v_0}{D} + I_{max}(1 - B)} \tag{17}$$

The partial derivative of ΔU with respect to I_{max} is

$$\partial \Delta U / \partial I_{max} = \frac{A B C_{av} v_0{}^2}{D[\frac{B v_0}{D} + I_{max}(1 - B)]^2} \tag{18}$$

When $(2 - \frac{r_0 v_0}{bD}) > 0$, $\dfrac{\left(\frac{r_1}{r_0}\right)^{\left(2-\frac{r_0 v_0}{bD}\right)}-1}{\left(\frac{r_1}{r_0}\right)^2-1} > 0$ because $r_1 > r_0$, and $\left(\dfrac{2}{2-\frac{r_0 v_0}{bD}}\right) > 0$. Therefore

$$B = \left(\frac{2}{2-\frac{r_0 v_0}{bD}}\right)\frac{\left(\frac{r_1}{r_0}\right)^{\left(2-\frac{r_0 v_0}{bD}\right)}-1}{\left(\frac{r_1}{r_0}\right)^2-1} > 0. \text{ When } \left(2 - \frac{r_0 v_0}{bD}\right) < 0, \frac{\left(\frac{r_1}{r_0}\right)^{\left(2-\frac{r_0 v_0}{bD}\right)}-1}{\left(\frac{r_1}{r_0}\right)^2-1} < 0 \text{ and } \left(\frac{2}{2-\frac{r_0 v_0}{bD}}\right) < 0.$$

Therefore B is positive as well. Because $A = 2\pi r_0 L_v \Delta t > 0$, $D = \dfrac{1}{K_m + C_{L0} - C_{min}} > 0$, $C_{av} > 0$, $B > 0$, the partial derivative $\partial \Delta U / \partial I_{max}$ (equation 18) is always positive, indicating that the function ΔU is monotonically increasing. That is, ΔU increases as I_{max} increases. Since the total amount of nutrient uptake is obtained by summing ΔU at each time interval, the total amount of nutrient uptake calculated this way increases as I_{max} increases. The structure of SSAND and PCATS is more complex. But this simple calculation indicates that the negative influence by I_{max} may be an artifact in the development of SSAND and PCATS.

Multiple dimensional sensitivity analysis

Figure 8 shows the relationship of simulated uptake to nutrient concentration in the soil solution (C_{Li}), which increases along the x-axis of each graph for both models. Each graph shows the results at a fixed level of root growth rate (k). The y-axis shows the simulated uptake in µmol, while the x-axis covers the range of C_{Li} values, and on each graph there are five different lines, one for each level of volumetric soil moisture (θ). Thus each line represents the change in uptake at given θ and k, with increasing C_{Li}. Each group of 5 graphs shows the results for a particular mechanistic model. The graphs are arranged such that k increases from the top row to the bottom. In general, uptake increases with C_{Li} until it reaches its maximum at high C_{Li}. Comparison of the five lines on each graph reveals that with those with a higher θ show the strongest response to increasing C_{Li}. But at high levels of C_{Li}, an increased θ does not produce any differences in uptake. At low C_{Li}, the uptake is strongly reduced. Comparison of graphs in the same row shows the effect of changing k. At low k, the maximal simulated uptake is strongly reduced. The maximal simulated uptake increases proportionally as k increases. If the simulated uptake by both models is fitted to a linear regression, the regression equations are similar. For example, if U_M (µmol) represents maximal simulated uptake, the equation for NST 3.0 is
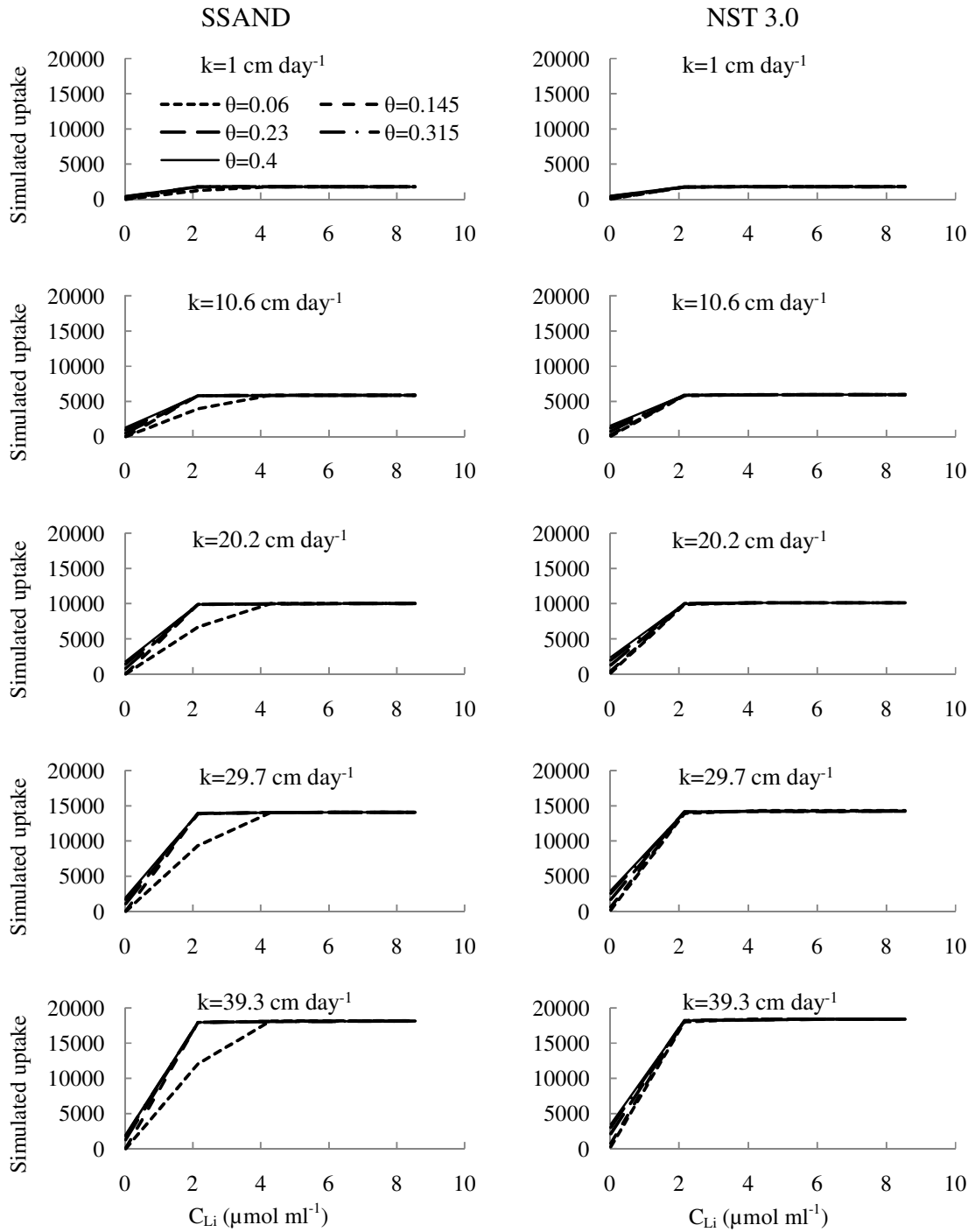
$$U_M = 433k + 1356.$$

Figure 8. Response surface from a multiple dimensional sensitivity analysis of SSAND and NST 3.0 using five levels of potassium concentration in the soil solution (C_{Li}), five levels of volumetric soil moisture (θ), and five levels of root growth rate (k). Other parameter values remained as listed in Table 6 for loblolly pine (Kelly et al. 1992). The unit of simulated uptake is µmol.

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Figure 9 shows the relationship of the same parameters used in the multiple dimensional sensitivity analysis depicted in Figure 8 in another way. In this case the x-axis covers the range in θ values and each graph represents a change in the C_{Li} value. The graphs of simulated uptake at higher C_{Li} values were not included in Figure 9 because for each k, the simulated uptake at the higher C_{Li} were the same as the uptake at $C_{Li}=2.156$ µmol ml^{-1} with a high θ. When C_{Li} is low (0.028 µmol ml^{-1}), SSAND produces lower estimates than NST 3.0. For example, when C_{Li} is 0.028 µmol ml^{-1} and θ is 0.06, the predicted potassium uptake by SSAND is less than 0.1 µmol, while uptake simulated by NST 3.0 ranges from 24 to 258 µmol. When C_{Li} is increased to 2.156 µmol ml^{-1}, the increase in θ did not lead to a significant change in simulated uptake by NST 3.0, but the uptake simulated by SSAND is significantly reduced at low θ (Figures 8 and 9). It seems that SSAND is more sensitive to θ, as was indicated in the one dimensional sensitivity analysis as well. However, the multiple dimensional sensitivity analysis also indicates the influence of θ on the SSAND simulation is only valid when C_{Li} is low (Figure 9).

Because the transient state model with a numerical solution is assumed to be more accurate than the steady state model (Smethurst and Comerford 1993b; Smethurst et al. 2004), the performance of SSAND can be evaluated by comparing its simulated results with those of NST 3.0 in our multiple dimensional sensitivity analysis. As shown in Figure 9, the predicted uptake by SSAND is lower than that of NST 3.0 before the simulations reach their maximums (an example is given in Figure 10). Given this underestimate, and the inability of SSAND to predict phosphorus uptake in the hybrid poplar study, it is suspected that SSAND is less able to predict uptake accurately when the supply of nutrients by the soil cannot meet the plant's needs as defined by the uptake kinetics parameters.

Conclusions

In summary, NST 3.0, SSAND, and PCATS differ both in predictive accuracy and model behavior. PCATS successfully predicted nitrate uptake, NST 3.0 predicted phosphorus uptake well, while SSAND underpredicted all nutrient uptake severely. Results were also diverse, indicating the need of reconsideration of the assumptions and solutions of the two mechanistic model categories. Although NST 3.0 and PCATS performed relatively well with some runs, the model predictions of the others failed to match the observation. The underestimates of many of
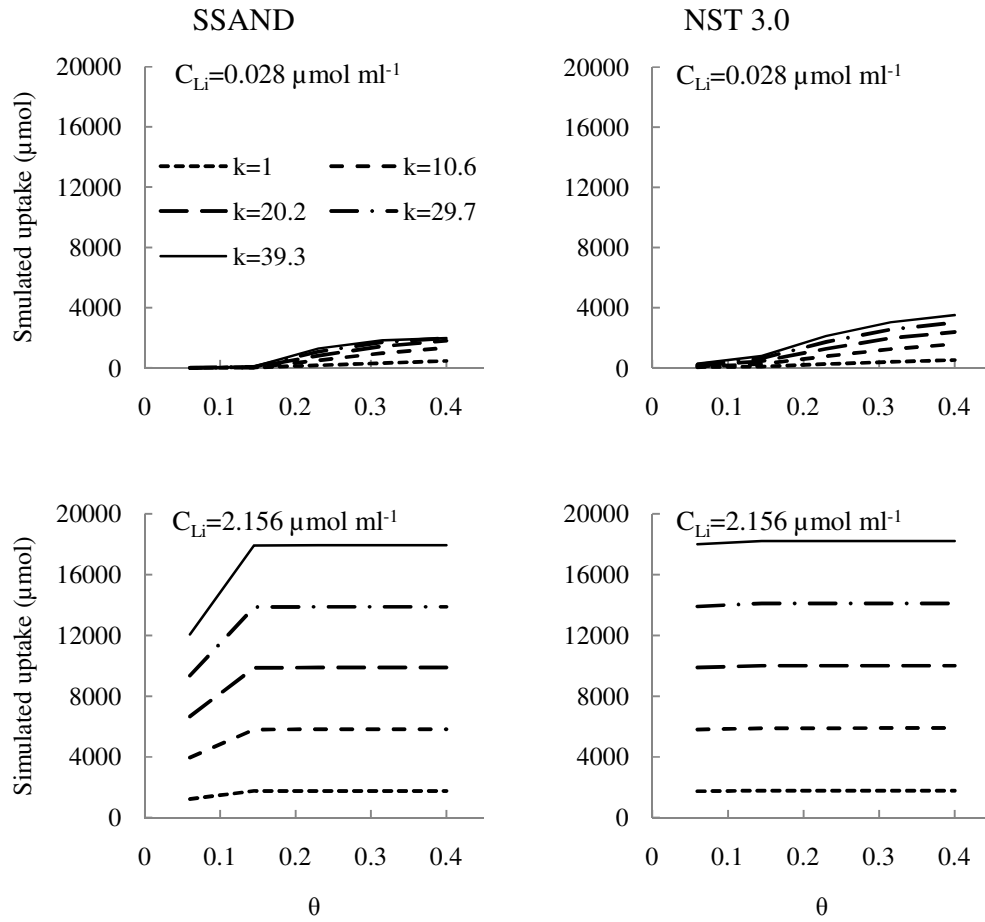
Figure 9. Response surface from a multiple dimensional sensitivity analysis of SSAND and NST 3.0 using two levels of potassium concentration in the soil solution (C_{Li}), five levels of volumetric soil moisture (θ), and five levels of root growth rate (k) with cm day^{-1} as the units. Other parameter values remained as listed in Table 6 for loblolly pine (Kelly et al. 1992).
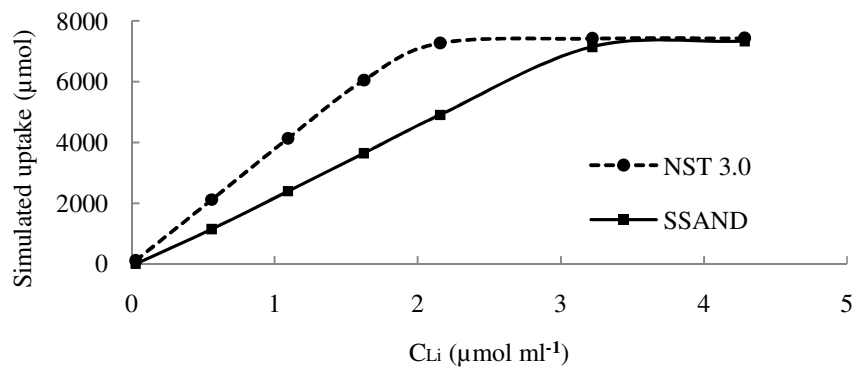
Figure 10. Simulated potassium uptake by SSAND and NST 3.0 with data taken from Kelly et al. (1992). The simulation was conducted with nutrient concentration in the soil solution (C_{Li}) changing from 0.028 to 4.284 µmol ml^{-1} while keeping other parameters unchanged.

the runs may be the results of running simulations without including the nutrient uptake by mycorrhizaes. But this alone cannot explain some successful simulations. Therefore, further studies that can produce representative datasets to evaluate the predictive accuracy against observed values for each model are needed for future model evaluation.

Both types of sensitivity analyses indicate that soil moisture (θ) plays an important role in uptake simulation when the nutrient concentration in the soil solution (C_{Li}) is low. This has not been noted in previous studies. Under low-nutrient-supply scenarios, I_{max} can influence the predictions of SSAND and PCATS negatively, and the uptake predictions of SSAND are generally lower than those of NST 3.0. We suspect that these are artifacts of the steady state models and further studies are needed to improve their ability to represent nutrient uptake under low-nutrient-supply scenarios.

In the process of soil exploration and nutrient uptake by plant roots, the influence of rhizospheric effects such as differences in rhizosphere pH and redox potential are important (Gillespie and Pope 1990; Marschner 1995). The three mechanistic nutrient uptake models do not include routines to describe such subprocesses except for the effects of mycorrhizaes. Because these effects are probably not negligible when the models are applied to longer growth periods and lower soil nutrient supply situations that are more typical of woody species, further studies to incorporate important rhizospheric effects other than mycorrhizae are suggested.

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