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Analytical Model for Zinc Uptake by Root System of *Thlaspi caerulescens*

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(*Received May 2, 2005 and accepted July 26, 2005*)

To develop future phytoextraction technologies, models describing the process of phytoextraction are necessary. In this paper we have developed an analytical model of zinc uptake by the growing root system of *Thlaspi caerulescens*, which includes zinc flow by convection and dispersion in soil, the growth of root system, and the total zinc flux to the root. Simulated results indicated that the model could quantitatively describe the zinc uptake process for *T. caerulescens*. Therefore, the model might help us to understand the quantitative characteristics of phytoextraction.

INTRODUCTION

The phenomenon of phytoextraction is performed in a complex plant–soil system. Phytoextraction of soil zinc by using *Thlaspi caerulescens* is dependent on not only genetic but also environmental characteristics. Zinc movement in the soil is governed by convection and dispersion flow. If the soil cannot supply sufficient zinc to the root surface, the capacity of hyperaccumulator will be limited (Whiting *et al.*, 2003). Moreover, the plant availability and the dynamic movement of zinc in the soil are influenced by physical, chemical and biological properties of the soil (Ernst, 1996; Whiting *et al.*, 2001).

Therefore, in the commercialization of phytoextraction technology, mathematical models are needed to evaluate the economic viability, to predict optimal metal removal rates, and to simulate plant physiological processes with physical, chemical and biological changes in plant–soil systems. Whiting *et al.* (2003) applied a solute transfer model (Baldwin *et al.*, 1973) to predict that the soil can supply zinc to the root of *T. caerulescens* at a sufficient rate for maximal phytoextraction. This model includes plant parameters like root density and rate of uptake, and it also contains parameters of zinc movement such as effective diffusion coefficient of zinc in soil, zinc buffer power of the soil, water flux from the soil to the root surface, etc. However, the model does not consider the root distribution and morphology of the plant. It has been reported by Schwartz *et al.* (1999) that the roots of *T. caerulescens* exhibited high affinity for soil containing zinc with high concentrations. This means the root distribution and morphology of *T. caerulescens* are important factors in phytoextraction which cannot be neglected.

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In this study, we developed a zinc uptake model to describe the soil zinc uptake by growing root system of *T. caerulescens* in the zinc phytoextraction.

MODEL DEVELOPMENT

Root growth model of *Thlaspi caerulescens*

Root branching structure develops when roots emerge from the seed, form lateral branches, and from their side. These lateral branches will in turn develop branches of their own. The branching occurs in the middle part of the root since non–branching regions exist near the base and tip of the roots. These non–branching regions develop as a result of root internal hormones, although the exact biochemical mechanism of their formation still remains unknown. Typically, the roots emerging from the seed, the zero order, are thickest in the system, and they connect to the stem of the plant. The higher lateral branch order, the smaller the radius of the branches becomes.

The surface of roots consists of epidermal cells. Some of those epidermal cells form extrusions into the soil, known as root hairs. Root hairs are transformations of the root surface cells and the mechanism of nutrient uptake by them seems to be similar to the uptake at the root surface. However, due to their small radius and high density, they may make a large contribution to the nutrient uptake.

To develop the model of zinc uptake, we need the information of the root size distribution. We assumed that the higher order roots are created by branching from the lower order roots. The frequency of branching, i.e., creation of higher order root, is dependent on the length of the lower order root.

Roots of *T. caerulescens* have typically 3 or 4 orders. The branches which emerge from the seed are called zero order branches, and the rest are called higher order branches. Roots of *T. caerulescens* also have root hairs emerged from the root surface cells. Due to their small radius and high density, root hairs have considerable root surface area and play an important role in zinc uptake. Therefore, the growth of zero order branches, first order branches, second order branches, and root hairs was considered in this study.

The root development of *T. caerulescens* can be described by a simple algebraic model derived by Hackett and Ross (1972), which gives the numbers and lengths of root members of different orders in terms of time:

$$N_0 = 1 \tag{1}$$
$$N_1 = R_0 Q_1 (T - T_1) \quad T > T_1 \tag{2}$$
$$N_2 = R_0 R_1 Q_1 Q_2 (T - T_2)^2 / 2 \quad T > T_2 \tag{3}$$

$$L_0 = V_0 (T - T_0) \quad T > T_0 \tag{4}$$
$$L_1 = R_0 Q_1 V_1 (T - T_1)^2 / 2 \quad T > T_1 \tag{5}$$
$$L_2 = R_0 R_1 Q_1 Q_2 V_2 (T - T_2)^3 / 6 \quad T > T_2 \tag{6}$$

where N_i ($i = 0$, 1, and 2) is the number of root members, L_i ($i = 0$, 1, and 2) is the length of root members, R_i ($i = 0$, 1, and 2) is the rate of extension of the branched region along a root member, Q_i ($i = 1$ and 2) is the density of branching, V_i ($i = 0$, 1, and 2) is the rate

of extension of root members, T is the time from initial wetting of the seed, and T_i ($i=0$, 1, and 2) is the time at which the first representative of each order of root appears.

The expressions above may be further simplified by assuming $R_i = V_i$.

The total number (N_h) and the total length (L_h) of root hair on the root can be expressed as:

$$N_h = L_0 Q_{h0} + L_1 Q_{h1} + L_2 Q_{h2} \tag{7}$$
$$L_h = N_h l_h \tag{8}$$

here Q_{hi} is the linear density of root hair on the ith order root ($i=0$, 1, and 2), and l_h is the length of a single root hair.

Hence, the effective length of each root member in the zinc uptake can be expressed as:

$$L_{0E} = (L_{0A} + L_{0B})/2 \tag{9}$$
$$L_{1E} = [(L_{1A} + (L_{1A}L_{1B})^{1/2} + L_{1B}]/3 \tag{10}$$
$$L_{2E} = [(L_{2A} + (L^2_{2A}L_{2B} + L_{2A}L^2_{2B})^{1/3} + L_{2B}]/4 \tag{11}$$

where L_{iE} ($i=0$, 1, and 2) is the effective length of root members, L_{iB} ($i=0$, 1, and 2) is the length of root members before zinc treatment, and L_{iA} ($i=0$, 1, and 2) is the length of root members after zinc treatment.

The effective length of root hair can be written as:

$$L_{hE} = (L_{0E}Q_{h0} + L_{1E}Q_{h1} + L_{2E}Q_{h2}) l_h \tag{12}$$

here Q_{hi} is the linear density of root hair on the ith order root, and l_h is the length of a single root hair ($i=0$, 1, and 2).

Zinc transport near root surface

Zinc uptake by roots can be described as a nutrient uptake model of plant. The nutrient uptake by roots is considered to occur in only liquid phase of the soil. We assumed that the soil is homogeneous, isotropic, and water saturated, and that the changes in the moisture condition are negligible. As in the classical models, the effect of root exudates, microbial activity, mycorrhizae etc. on the plant nutrient uptake and nutrient movement in the soil was neglected. The movement of nutrient to the root surface can take place by convection due to water uptake by the plant, and by dispersion of nutrient ions in the soil pore water. Zinc uptake by a single cylindrical root can be described using the model derived by Nye and Marriott (1969):

$$\frac{\partial C}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left(rD \frac{\partial C}{\partial r} + \frac{v_0 r_0}{b} C \right) \tag{13}$$

where r is the radial distance from the root axis, r_0 is the root radius, C is zinc concentration in soil solution, v_0 is the inward flux of water at the root surface, D is the dispersion coefficient (considered constant) in the soil, b is the differential buffer power (i.e., $b = dC_d/dC_l$, where C_d is the total concentration of diffusible solute, C_l is the concentration of solute in soil solution.)(Baldwin *et al.*, 1973), and t is time of uptake.

The initial conditions are:

$$C=C_s, \ t=0, \ r>r_0,\qquad\qquad\qquad\qquad(14)$$

where C_s is the initial zinc concentration in the soil solution.

Metal ions cannot move freely across the cellular membranes, which are lipophilic structures. Therefore, ion transport into cells must be mediated with membrane proteins having transport functions, generically known as transporters. These transporters are characterized by certain kinetic parameters, such as transport capacity (maximum catalytic rates: I_{max}) and affinity for ion (substrate affinities: K_m). I_{max} measures the maximum rate of ion transport across the cellular membranes. K_m measures transporter affinity for specific ion and represents the ion concentration in the external solution at which the transport rate equals $I_{max}/2$. A low K_m value, high affinity, indicates that high levels of ions are transported into cells, even at low external ion concentration. By studying the kinetic parameters, K_m and I_{max}, insights to specificity and selectivity of the transport system can be gained.

As proved by some researchers, zinc uptake by *Thlaspi caerulescens* takes place through transporters (Pence *et al.*, 2000; Assunção *et al.*, 2001). It can be described by Michaelis–Menten kinetics:

$$I=\frac{I_{max}C_0}{K_m+C_0}\qquad\qquad\qquad\qquad(15)$$

where I is rate of the root influx, I_{max} is the maximum influx rate, K_m is the value of the concentration at which $I=I_{max}/2$, C_0 is the zinc concentration at the root surface.

Eq. (13) is subjected to two boundary conditions as described by Nye and Marriott (1969). The first is:

$$Db\ \frac{\partial C}{\partial r}+v_0C=\frac{I_{max}C_0}{K_m+C}\quad \text{for}\quad t>0, r=r_0\qquad\qquad(16)$$

If we assume zinc concentration in soil solution is low, Eq. (16) reduces to:

$$Db\ \frac{\partial C}{\partial r}+v_0C=k_mC\qquad \text{for}\qquad t>0, r=r_0\qquad\qquad(17a)$$

where $k_m=I_{max}/K_m$.

If we assume zinc concentration in soil solution is high, then Eq. (16) reduces to:

$$Db\ \frac{\partial C}{\partial r}+v_0C=I_{max}\qquad \text{for}\qquad t>0, r=r_0\qquad\qquad(17b)$$

The second boundary condition is:

$$Db\ \frac{\partial C}{\partial r}+v_1C=0\qquad \text{for}\qquad t>0, r=r_1$$

where r_1 is the radius of a cylinder coaxial that is far from the root axis, v_1 is the inward flux of water at r_1. Here, it is assumed that no nutrient passes through the outer cylinder wall and yet water is allowed to pass through (Cushman, 1979a). For conservation of

water,

$$2\pi r_0 v_0 = 2\pi r_1 v_1.$$

Thus, the outer boundary condition considering inter–root competition for nutrient may be expressed as:

$$Db\,\frac{\partial C}{\partial r} + \frac{r_0}{r_1}\,v_0 C = 0 \qquad \text{for} \quad t > 0, r = r_1. \tag{18}$$

The nondimensionalization of variables can be performed following Cushman's (1979a) method:

$$w = t(D/r_0^2) \tag{19a}$$
$$z = r/r_0 \tag{19b}$$
$$X(z, w) = 1 - C(r, t)/C_s \tag{19c}$$
$$u = -r_0 v_0 / 2Db \tag{19d}$$
$$p = I_{max}/k_m C_s \tag{19e}$$
$$\beta = k_m / v_0 \tag{19f}$$
$$a = r_1 / r_0 \tag{19g}$$

Therefore, Eqs. (13), (14), (17a), (17b), and (18) become:

$$\frac{\partial X}{\partial w} = \frac{\partial^2 X}{\partial z^2} + \frac{1}{z}(1 - 2\mu)\frac{\partial X}{\partial z} \tag{20}$$

$$X = 0 \qquad \text{for} \quad w = 0, 1 < z < a \tag{21}$$

$$\frac{\partial X}{\partial z} = 2\mu(X-1)(1-\beta) \qquad \text{for} \quad w > 0, z = 1 \tag{22}$$

$$\frac{\partial X}{\partial z} = 2\mu[(X-1) + \beta p] \qquad \text{for} \quad w > 0, z = 1 \tag{23}$$

$$\frac{\partial X}{\partial z} = \frac{2\mu}{a}(X-1) \qquad \text{for} \quad w > 0, z = a \tag{24}$$

respectively.

Assuming $X(z, w)$ can be expressed as $X(z, w) = W(w)Z(z)$, thus two ordinary differential equations may be obtained from Eq. (20) :

$$W' + \lambda^2 W = 0 \tag{25}$$

and

$$Z'' + \frac{1}{z}(1 - 2\mu)Z' + \lambda^2 Z = 0 \tag{26}$$

The solutions of Eq. (25) and (26) are:

$$W(w) = A_1 \exp(-\lambda^2 w) \tag{27}$$

and

$$Z(z) = A_2 z^u J_u(\lambda z) + A_3 z^u Y_u(\lambda z) \tag{28}$$

Here A_1, A_2, A_3, and λ are constants. J_u and Y_u are Bessel functions of the first and second kind, respectively, which are expressed as:

$$J_u(\lambda z) = \sum_{k=0}^{\infty} \frac{(-1)^k (\lambda z/2)^{u+2k}}{k! \, \Gamma(u+k+1)} \tag{29}$$

$$J_{-u}(\lambda z) = \sum_{k=0}^{\infty} \frac{(-1)^k (\lambda z/2)^{-u+2k}}{k! \, \Gamma(-u+k+1)} \tag{30}$$

$$Y_u(\lambda z) = \frac{J_u(\lambda z)\cos(u\pi) - J_{-u}(\lambda z)}{\sin(u\pi)} \tag{31}$$

where $\Gamma(u+k+1)$ and $\Gamma(-u+k+1)$ are gamma functions. Therefore, the general solution of Eq. (20) can be written as:

$$X(z, w) = A_1 \exp(-\lambda^2 w)[A_2 z^u J_u(\lambda z) + A_3 z^u Y_u(\lambda z)] \tag{32}$$

As inter–root competition is considered, we can obtain a specific solution $X(z,w) = 1$ when $C(r, t) = 0$, which means zinc is completely depleted. Hence, Eq. (32) can be expressed as:

$$X(z, w) = \sum_{n=0}^{\infty} A_n z^u B_u(\lambda_n, z) \exp(-\lambda_n^2 w) + 1 \tag{33}$$

Where

$$B_u(\lambda_n, z, \beta) = [\lambda_n Y_{u-1}(\lambda_n) - 2u(1-\beta)Y_u(\lambda_n)]J_u(\lambda_n z)$$
$$-[\lambda_n J_{u-1}(\lambda_n) - 2u(1-\beta)Ju(\lambda_n)]Y_u(\lambda_n z) \tag{34}$$

For inter root competition, λ_n satisfy

$$[\lambda a J_{u-1}(\lambda a) - 2u J_u(\lambda a)]\lambda Y_{u-1}(\lambda) - 2u(1-\beta)Y_u(\lambda)]$$
$$-[\lambda a Y_{u-1}(\lambda a) - 2u Y_u(\lambda a)][\lambda J u_{-1}(\lambda) - 2u(1-\beta)Ju(\lambda)] = 0 \tag{35}$$

To satisfy the initial condition,

$$\sum_{n=0}^{\infty} A_n z^u B_u(\lambda_n, z) = -1$$

is needed. A_n can be obtained as:

$$A_n = -\int_1^a z^{1-u} B_u(\lambda_n, z) \mathrm{d}z / \int_1^a z B_u^2(\lambda_n, z) \mathrm{d}z \tag{36}$$

Total zinc uptake by the root system of *Thlaspi caerulescens*

If we assume that all the root members of ith order root have the same radius. The total zinc uptake can be written as:

$$F_{\text{Total}} = \sum_{i=0}^{2} \int_{T_s}^{T} 2\pi\rho_i L_i(t) F_i(t) \mathrm{d}t + \int_{T_s}^{T} 2\pi\rho_h L_h(t) F_h(t) \mathrm{d}t \tag{37}$$

where ρ_i is the radius of the root members of ith order root, ρ_h is the radius of a single root hair, T is the time from initial wetting of the seed, T_s is the time at which the zinc treatment starts, $F_i(t)$ is the flux of zinc at the root surface, and $F_h(t)$ is the flux of zinc at the root hair surface. $L_i(t)$ and $L_h(t)$ are the length of ith order root and the root hair respectively, which are the functions of time ($i=0$, 1, and 2).

From Equation (17a) and (17b), when soil zinc concentration is low, the flux at the root can be written as:

$$F_i(t) = k_m C \qquad \text{at} \qquad r = r_0 \tag{38}$$

and at high soil zinc concentration, it can be

$$F_i(t) = I_{\max} \qquad \text{at} \qquad r = r_0 \tag{39}$$

In nondimensional variables, we can obtain:

$$F_i(t) = k_m C_0[1 - X(z, w)] \qquad \text{at} \qquad z = 1 \tag{40}$$

$$F_i(t) = k_m C_0 p \qquad \text{at} \qquad z = 1 \tag{41}$$

Therefore, when the soil zinc concentration is low, the total flux F^L_{Total} of zinc at root surface of *T. caerulescens* can be expressed as:

$$F^L_{\text{Total}} = \sum_{i=0}^{2} \frac{2\pi k_m C_0 \rho_i^3 L_{iE}}{D} \int_{ws}^{w} [1 - X_i(1, w)] \mathrm{d}w$$

$$+ \frac{2\pi k_m C_0 \rho_h^3 L_{hE}}{D} \int_{ws}^{w} [1 - X_h(1, w)] \mathrm{d}w \tag{42}$$

and when the soil zinc concentration is high, the total flux F^H_{Total} is written as:

$$F^H_{\text{Total}} = \sum_{i=0}^{2} \frac{2\pi k_m C_0 \rho_i^3 L_{iE} \rho_i (w - w_s)}{D}$$

$$+ \frac{2\pi k_m C_0 \rho_h^3 L_{hE} \rho_h (w - w_s)}{D} \tag{43}$$

where L_{iE} is the effective length of ith order root and L_{hE} is the effective length of the root

hair in zinc treatment. ($i=0, 1,$ and 2)

EVALUATION OF THE MODEL

Measurements of water–soluble zinc concentrations and soil pH values

Water–soluble zinc in vermiculite sample was extracted by mixing the samples with deionized water at a vermiculite/water ratio of 1:8 (g ml⁻¹) in 50–mL centrifuge tubes. A 24–hour equilibration was performed at room temperature, with shaking samples (110 oscillations per min) on a horizontal shaker for one hour every 6 hours. Samples were centrifuged (2000 rpm, 15 min) and filtered. Zinc concentrations of filtrate were determined using a fluorescent X–ray (FXR) analyzer (EDX–800, Shimadzu) at the Center of Advanced Instrumental Analysis, Kyushu University (Japan), and water–soluble zinc concentrations in vermiculite were calculated. The resulted relationship between water–soluble zinc and total zinc is shown in Fig. 1.
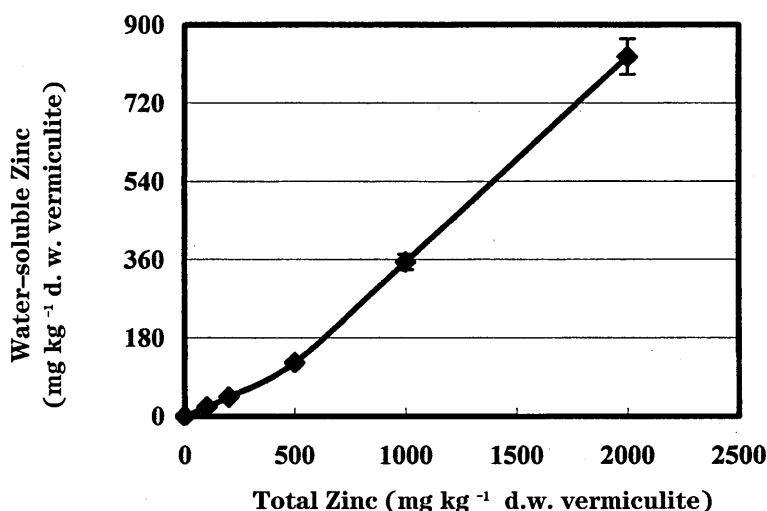

Fig. 1. The relationship between water–soluble zinc and total zinc in vermiculite.

Determination of growth parameters of root system

T. caerulescens was germinated by placing seeds on the filter paper that was kept moist in the 0.5 concentrated Otsuka nutrient solution [940 of $Ca(NO_3)_2 \cdot 4H_2O$, 810 of KNO_3, 490 of $MgSO_4 \cdot 7H_2O$, 150 of $NH_4H_2PO_4$, 22.62 of Fe–EDTA, 2.86 of H_3BO_3, 1.81 of $MnCl_2 \cdot 4H_2O$, 0.22 of $ZnSO_4 \cdot 7H_2O$, 0.08 of $CuSO_4 \cdot 5H_2O$, and 0.025 mg L^{-1} of $Na_2MoO_4 \cdot 2H_2O$]. Fifteen days later, seedlings of *T. caerulescens* were planted for each pot containing 250 g of vermiculite. Basal fertilizer was also applied by 100 mg N kg⁻¹ dry vermiculite as

NH_4NO_3, and 80 mg P kg^{-1} and 100 mg K kg^{-1} as KH_2PO_4. Zinc was added as $ZnSO_4$ solution. Zinc treatments were 0, 100, 200, 500, 1000, and 2000 mg kg^{-1}. The vermiculite moisture content was approximately maintained at 1.5 g g^{-1} (water/vermiculite). The pH value was initially set at 6.00. The plants were grown in the glass room, in which the temperature was controlled at 25 °C in the daytime and 20 °C at night and the relative humidity at 70%. Plants were harvested at 5, 10, 15, 20, 25, and 30th day after the transplanting. Number and length of root members for respective root order were measured. The result is shown in Table 1.

Table 1. The number and length of root members of *Thlaspi caerulescens*.

Growth Measurement		Time from Seeding (day)						
		15	20	25	30	35	40	45
Zero	Average Number	1	1	1	1	1	1	1
Order	Average Length (mm)	39	53	65	80	94	108	123
First	Average Number	8	9	11	14	16	19	21
Order	Average Length (mm)	6	11	15	18	22	26	30
Second	Average Number	5	11	20	31	46	65	87
Order	Average Length (mm)	3	5	8	10	13	15	17

Eq. (1) to (12) were employed to calculate the rate of extension of the branched region along a root member (R_i) ($i=0$, 1, and 2), the density of branching (Q_i) ($i=1$ and 2), and the rate of extension of root members (V_i) ($i=0$, 1, and 2) for different culture periods were determined by using the experimental data. The rate of extension and the density of branch are the functions of time, which were shown in Fig. 2 and Fig. 3. Q_1 and Q_2 represent the density of first order and second order respectively. V_0, V_1, and V_2 are the extension rate of zero order, first order, and second order respectively. Here, we assume that R_i is equal to V_i. T is the time from initial wetting of the seed. The time at which the root of the zero order appeared was the third day. For the first order, it was the fifth day. And for the second order, it was the eighth day.

In the pot culture experiment of *T. caerulescens*, the lengths of root members of different orders were calculated by using the rate of extension of the branched region along a root member, the density of branching, and the rate of extension of root members obtained from Fig. 2 and Fig. 3 (see the dashed lines). The growth parameters are listed in Table 2, where R_i ($i=0$, 1, and 2) is the rate of extension of the branched region along a root member, Q_i ($i=1$ and 2) is the density of branching, and V_i ($i=0$, 1, and 2) is the rate of extension of root members in pot culture experiment, T is the time from seeding, and T_i is the time at which the first representative of each order of root appeared ($i=0$, 1, and 2). The length of a single root hair (l_h) is assumed to be 1 mm. The numbers of root hair in the unit length (per mm) of zero order, first order, and second order are 62, 47, and 24 respectively. The length and average radius of each order of the plant root system are shown in Table 3.
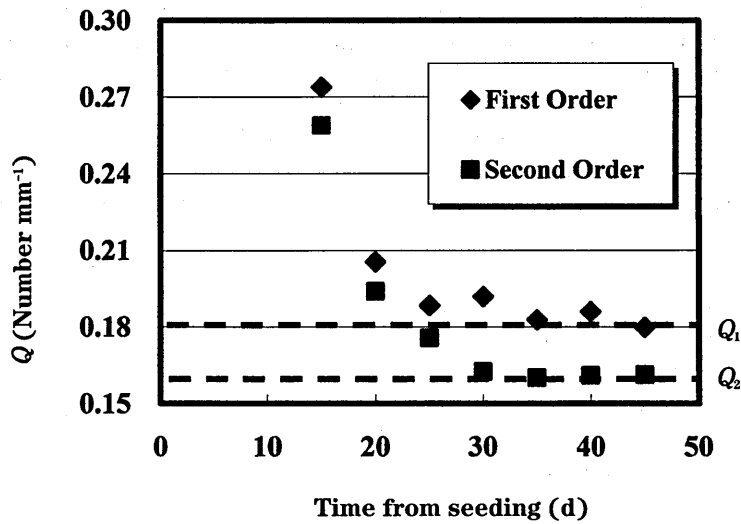
Fig. 2. The density of branching as a function of time.
Dashed line indicates the value that is used in the calculation.
Diamonds and squares are experimental results.
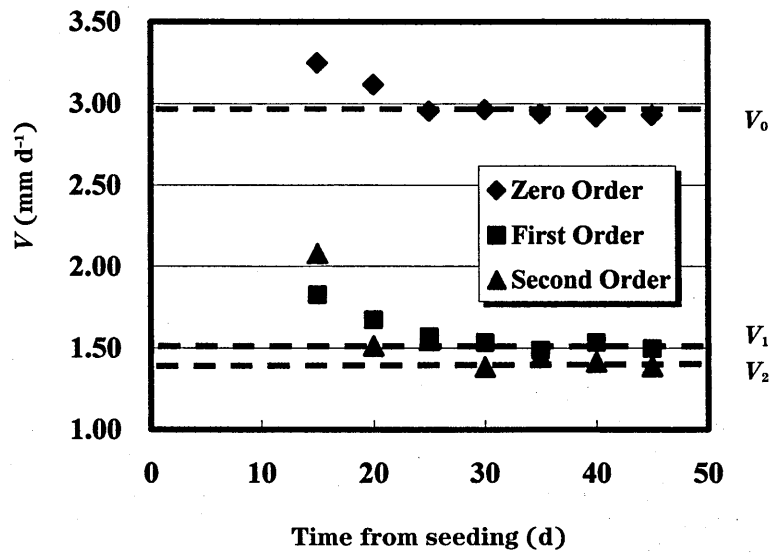
Fig. 3. The extension rate as a function of time.
Dashed line indicates the value that is used in the calculation.
Diamonds, squares, and triangles are experimental results.

Table 2. The growth parameters of the root members of *Thlaspi caerulescens*.

Parameter	T_i (day)	Q_i (Number mm^{-1})	$R_i = V_i$ (mm d^{-1})
Zero Order	3	#	2.92
First Order	5	0.18	1.50
Second Order	8	0.16	1.40

Table 3. The length and the radius of each root member of *Thlaspi caerulescens*.

Parameter	L_E(mm)[a]	ρ (mm)
Zero Order	269	1.8
First Order	3388	1.0
Second Order	21660	0.5
Root Hair	695754	0.01[b]

a. L_E is the effective length and ρ is radius of each root member.
b. The radius of the root hair was assumed as a constant the value of 0.01 mm.

Test of equations

The total zinc uptake model has been derived by Eq. (42). The solution contains infinite series of the Bessel functions $J_u(x)$ and $Y_u(x)$, where $\mu = -r_0v_0/2Db$ as defined by Eq. (19d). $J_{-n-1/2}$ and $J_{n+1/2}$ can be written as products of trigonometric functions (sines and cosines) and powers of $1/x^{1/2}$ (Watson, 1966). And it was given by Mclachlan (1971):

$$J_{-n-1/2}(x) = (-1)^n J_{n+1/2}(x) \tag{44}$$
$$J_{-1/2}(x) = (2/\pi/x)^{1/2}\cos x \tag{45a}$$
$$Y_{-1/2}(x) = (2/\pi/x)^{1/2}\sin x \tag{45b}$$
$$J_{-3/2}(x) = (2/\pi/x)^{1/2}[-\sin x - \cos x/x] \tag{45c}$$
$$Y_{-3/2}(x) = (2/\pi/x)^{1/2}[-\sin x/x + \cos x] \tag{45d}$$
$$J_{-5/2}(x) = (2/\pi/x)^{1/2}[(3/x)\sin x + (3/x^2-1)\cos x] \tag{45e}$$
$$Y_{-5/2}(x) = (2/\pi/x)^{1/2}[(3/x^2-1)\sin x - (3/x)\cos x] \tag{45f}$$

and etc.

Assuming $\mu = -1/2$, i.e., $r_0v_0/Db = 1$, we can rewritten Eqs. (34), (36), and (33) as:

$$B_u(\lambda_n, z) = 2(\pi\lambda_n z^{1/2})^{-1}\{\lambda_n\cos[\lambda_n(1-z)] - \beta\sin[\lambda_n(1-z)]\} \tag{46}$$

$$A_n = -(\pi\lambda_n/2)\int_1^a z\{\lambda_n\cos[\lambda_n(1-z)] - \beta\sin[\lambda_n(1-z)]\}dz/ \tag{47}$$

$$\int_1^a \{\lambda_n\cos[\lambda_n(1-z)] - \beta\sin[\lambda_n(1-z)]\}^2 dz$$

$$X(z, w) = (2/\pi/z)\sum_{n=0}^{\infty} A_n\{\lambda_n\cos[\lambda_n(1-z)] - \beta\sin[\lambda_n(1-z)]\}\exp(-\lambda_n^2 w)/\lambda_n + 1 \tag{48}$$

As $z=1$, Eqs. (46), (47), and (42) can be rewritten as:

$$B_u(\lambda_n, 1)=2/\pi \tag{46'}$$
$$A_n=\pi\lambda_n/2 \tag{47'}$$

And

$$F^{L}{}_{Total}=\sum_{i=0}^{2}\frac{2\pi k_m C_0 \rho_i^3 L_{iE}}{D}\int_{ws}^{w}[(\pi/w)^{1/2}/2]dw$$

$$+\frac{2\pi k_m C_0 \rho_h^3 L_{hE}}{D}\int_{ws}^{w}[(\pi/w)^{1/2}/2]dw \tag{49}$$

By using Eq. (19a), we can rewrite respective Eq. (49) and (43) as:

$$F^{L}{}_{Total}=\sum_{i=0}^{2}\frac{2\pi^{3/2}k_m C_0 \rho_i^2 L_{iE}}{D^{1/2}}[(T)^{1/2}-(T_s)^{1/2}]$$

$$+\frac{2\pi^{3/2}k_m C_0 \rho_h^2 L_{hE}}{D^{1/2}}[(T)^{1/2}-(T_s)^{1/2}] \tag{50}$$

and

$$F^{H}{}_{Total}=\sum_{i=0}^{2}2\pi I_{max}\rho_i L_{iE}(T-T_s)$$

$$+2\pi I_{max}\rho_h L_{hE}(T-T_s) \tag{51}$$

Hence, the total uptake by a single plant can be described by Eq. (50) or (51).

(A) *In the case of high concentration of zinc – the test of Eq. (51)*

When the zinc concentration of the soil is so high that the soil can supply zinc to the root of *T. caerulescens* at a sufficient rate for maximal phytoextraction, total zinc uptake is dependent on the area of the root surface and the maximum rate of ion transport across the cellular membranes, which is essentially resulted from the genetic factor. In this case, the total zinc uptake by *T. caerulescens* can be obtained from Eq. (51). Using the data of Lasat *et al.* (1996) [$V_{max}=0.27\mu$mol g^{-1}(fresh weight) h^{-1}, $K_m=8\mu$M], we calculated the maximum zinc uptake rate by *T. caerulescens* to be 53.21μmol d^{-1} m^{-2}. Here we use this value as the I_{max}. Parameters of the effective length (L_E) and the radius (ρ) of each root member were shown in Table 3. Ts and T were given as 35 d and 125 d, respectively. Hence, from Eq.s (51) we can obtain:

$$F^{H}{}_{Total}=42.58\,\text{mg pot}^{-1} \tag{52}$$

Compared with the experimental data (Table 4), this value is larger than the results from the experiments except that in zinc treatment of 2000 mg kg^{-1}. Theoretically, the result from Eq. (51) should be the maximum value of zinc accumulation. The error might be caused by the calculation of root growth parameters, in which only zero order, first order,

second order, and the root hair have been considered. However, further calculations revealed that the result calculated by Eq. (51) approximated to the average level (45.10 mg pot⁻¹) of zinc accumulated by *T. caerulescens* with zinc treatments of 1000 mg kg⁻¹ and 2000 mg kg⁻¹. This means Eq. (51) could be applied to estimate the zinc uptake by *T. caerulescens* when the soil zinc concentration is so high that the zinc influx at the root surface is in the saturate state.

Table 4. The amount of zinc accumulated by *Thlaspi caerulescens*.

Treatment (mg km⁻¹ d.w.)	0	100	200	500	1000	2000
Total Zinc Uptake (mg pot⁻¹)	0	3.37	10.67	22.36	39.54	50.65

(B) *In the case of low concentration of zinc – the test of Eq. (50)*

Zinc uptake by *T. caerulescens* is usually limited by the zinc supply of the soil, especially when the soil zinc concentration is low. In this case, total zinc uptake of the plant is not only dependent to the genetic factors, but also affected by the soil characteristics. In Eq. (50), both plant factor and medium factor have been considered. By using the same data of Lasat *et al.* (1996), as shown in (A), we can calculate k_m by the equation $k_m = I_{max}/K_m$. Hence, the value of k_m is 0.00665 m d⁻¹. We used the value of Shuman (1980) (0.311 × 10⁻⁸ m d⁻¹) as the dispersion coefficient of zinc (D), which had also been used by Whiting *et al.* (2003). We did not determine C_0 in Eq. (50), which is the zinc concentration at the root surface. By using the result calculated in the case of high concentration of zinc [Eq. (52)] and the data in Table 4, we obtained the zinc concentration in vermiculite C_{ws} of 1273.63 mg km⁻¹ d.w. vermiculite when the zinc influx at the root surface was in the saturate state. It can be assumed that C_0 is dependent on the water–soluble zinc in the vermiculite. Thus, we calculated C_0 as following:

$$C_0 = C_s \, C_w / C_{ws}$$

where C_s is the root surface concentration of zinc at which the zinc influx is in the saturate state, a value of 27 μM was used (Whiting *et al.*, 2003); C_w is the concentration of water–soluble zinc; and C_{ws} is the zinc concentration in vermiculite at which the zinc influx is in the saturate state (Fig. 1). Parameters of the effective length (L_E) and the radius (ρ) of each root member are shown in Table 3. T_s and T were given as 35 d and 125 d, respectively. Figure 4 shows the results obtained from the calculation and the experiment.

It is clear that there is an agreement between the results calculated by Eq. (50) and the experimental data at low soil zinc concentrations, while the errors are very large when we calculate the total zinc uptake of the plant by using Eq. (50) at high zinc concentration. This means Eq. (50) is suitable for predicting the total zinc uptake by *T. caerulescens* at relative low zinc concentrations.

DISSCUSSION

In this study, we have developed a model of zinc uptake by the growing root system
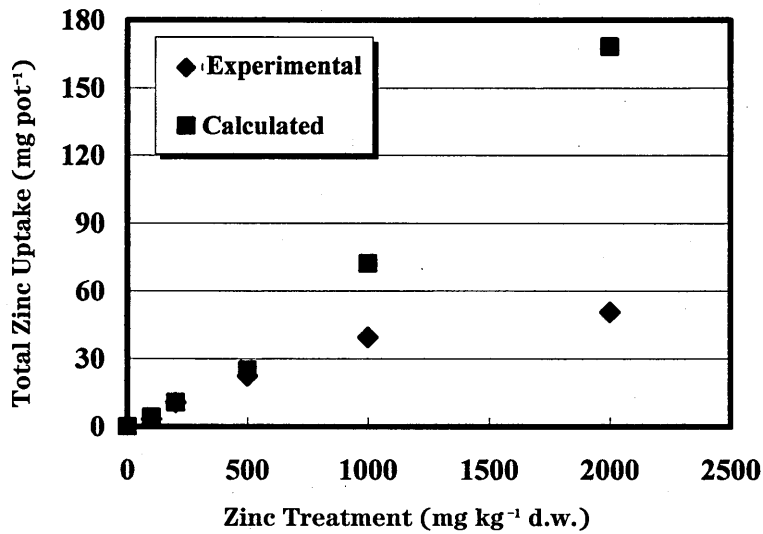
Fig. 4. Total zinc uptake at 125th day after seeding. The values were obtained from the experiments and calculation [Eq. (50)].
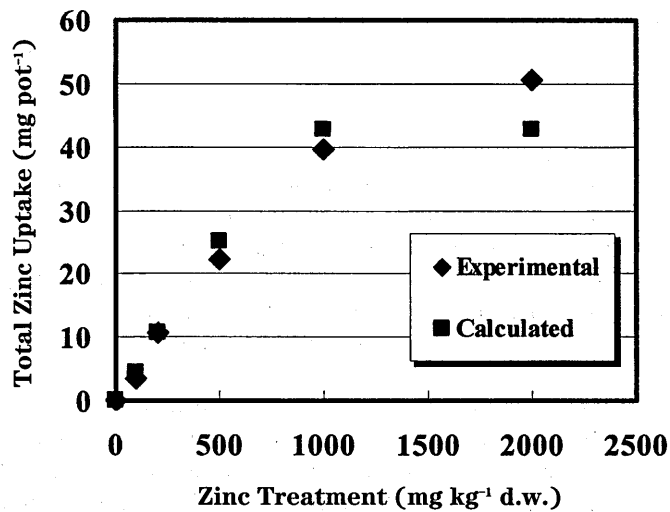

Fig. 5. Total zinc uptake at 125th day after seeding. The values were obtained from the experiments and the calculations [Eq. (50) and (51)].

of *T. caerulescens* and derived the computer solutions. The model includes soil zinc supply by diffusion and mass flow, the growth of root system, and the total zinc flux to the root. Tested against the experimental data, the model has given results in close agreement (Fig. 5).

For the calculated data in Figure 5, we used the results obtained from Eq. (50) in the case of relatively low concentrations of soil zinc ($\leq$500 mg kg^{-1} d.w.), while at relatively high concentrations of soil zinc (>500 mg kg^{-1} d.w.), the value calculated by Eq. (51) was used. The calculation error appeared in the case of high zinc concentrations. It might be caused by the calculation of growth parameters, in which less root orders were taken into account. Therefore, we should improve the evaluation method of root order for the effective use of Eq. (51).

Although the error exists, this model could be useful to simulate the zinc uptake by a growing root system of *T. caerulescens*, especially when the soil zinc concentrations are relatively low. The model can quantitatively describe the zinc accumulation in the growing processes in *T. caerulescens*, which is controlled by not only the genetic but also the environmental factors. The model is also helpful to predict the total zinc uptake by *T. caerulescens* in different zinc concentrations in soil. In addition, because relationships among the soil zinc supply, the growth of root system, and the total zinc flux to the root are considered, this model might be employed to optimize the future phytoextraction technologies.

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