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Analysis and use of cumulative nutrient uptake formulas in plant nutrition and the temporal-weight-averaged influx

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ABSTRACT

A generalized cumulative uptake formula of nutrient uptake by roots following our previous formula (Reginato-Tarzia, Comm. Soil Sci. and Plant., 33 (2002), 821-830) is developed. Cumulative nutrient uptake obtained by this formula is compared with the simulated results obtained by the Claassen and Barber (Claassen and Barber, Agronomy J., 68 (1976) 961–964) and Cushman (Cushman, Soil Sci. Soc., 43 (1979) 1087–1090) formulas. A mass balance is analyzed for the three formulas of cumulative nutrient uptake in order to decide which of them is correct. Moreover, the mass balance is also verified through a computational algorithm using data obtained from literature, and we compute the potassium (K) uptake for maize for low and high soil concentrations using the three mentioned formulas. The theoretical analysis shows that Claassen and Barber, and Cushman formulas do not verify, in general, the mass balance condition. The Claassen and Barber formula only verifies this condition when the influx is constant and root grows linearly. The Cushman formula verifies the mass balance when the influx is constant regardless of the law of root growth. Reginato and Tarzia formula always verifies the mass balance whatever be the representative functions for the influx and the law of root growth. Moreover, we propose a redefinition of the averaged influx from which the Williams formula (Williams, J. Scientific Res., 1 (1948) 333–361) can be deduced. We remark that Williams formula is a consequence of our definition of temporal-weight-averaged influx for all root growth law expressions. Also, we present a comparison of influx and cumulative uptake of cadmium (Cd) with data extracted from literature. Cumulative uptake is obtained through the Barber–Cushman model and our moving boundary model by using the redefinition of averaged influx on root surface and the correct cumulative uptake formula presented in this paper.

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cumulative nutrient uptake; mass balance; nutrient influx; Williams's formula

Introduction

Simulations of transport and nutrient uptake by roots generate a set of influxes data at the root–soilinterface. From these influxes, the cumulative nutrient uptake is calculated integrating on a variable the Claasen and Barber formula (1976)

$$U_{CB} = 2\pi s_o \ell(t_i) \int_{t_i}^{t_f} J(t)dt + 2\pi s_o \int_{t_i}^{t_f} \left[\int_{t_i}^{\tau} J(t)dt + \right] \dot{\ell}(\tau)d\tau, \qquad (1)$$

the Cushman formula (1979)

$$U_C = 2\pi s_o \ell(t_i) \int_{t_i}^{t_f} J(t)dt + 2\pi s_o \int_{t_i}^{t_f} \left[\int_{t_i}^{t_f-\tau} J(t)dt + \right] \dot{\ell}(\tau)d\tau, \qquad (2)$$

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and the Reginato and Tarzia formula (2002)

$$U_{RT} = 2\pi s_o \ell(t_i) \int_{t_i}^{t_f} J(t)dt + 2\pi s_o \int_{t_i}^{t_f} \left[\int_{\tau}^{t_f} J(t)dt + \right] \dot{\ell}(\tau)d\tau, \tag{3}$$

where t_i and t_f are the initial and final times, respectively, s_o is the root radius, $\ell_o$is the initial root length, J(t) is the influx on the root surface as a function of the time t and $\ell(t)$ is the rate of root growth as a function of time.

Depending on the used formula, a wide dispersion in the results can be obtained for the cumulative nutrient uptake. In order to show this fact, we will discuss which of the three formulas for cumulative nutrient uptake is the most appropriate with the corresponding efficiency. Prior to this analysis, a simplified formula of Eq. (3) for U_{RT} is obtained in the following manner:

$$\begin{aligned}
U_{RT} &= 2\pi s_o \ell(t_i) \int_{t_i}^{t_f} J(t)dt + 2\pi s_o \int_{t_i}^{t_f} \underbrace{\left[\int_{\tau}^{t_f} J(s)ds\right]}_{V} \underbrace{\dot{\ell}(\tau)}_{\dot{U}} d\tau \\
&= 2\pi s_o \ell(t_i) \int_{t_i}^{t_f} J(t)dt + 2\pi s_o \left[\ell(\tau)\left(\int_{\tau}^{t_f} J(s)ds\right)\Big|_{\tau=t_i}^{\tau=t_f} + \int_{t_i}^{t_f} J(t)\ell(t)dt\right] \\
&= 2\pi s_o \ell(t_i) \int_{t_i}^{t_f} J(t)dt + 2\pi s_o \left[0.\ell(t_f) - \ell(t_i)\left(\int_{t_i}^{t_f} J(t)dt\right) + \int_{t_i}^{t_f} J(t)\ell(t)d\tau\right] \\
&= 2\pi s_o \ell(t_i) \int_{t_i}^{t_f} J(t)dt - 2\pi s_o \ell(t_i) \int_{t_i}^{t_f} J(t)dt + 2\pi s_o \int_{t_i}^{t_f} J(t)\ell(t)d\tau \\
&= 2\pi s_o \int_{t_i}^{t_f} J(t)\ell(t)d\tau,
\end{aligned} \tag{4}$$

where the product $2\pi s_o J(t)\ell(t)$ represent the instantaneous nutrient uptake. The last formula (4) can also be obtained from basic physics principles owing to J(t) is the amount of nutrient by unit of time and unit of area that the root takes. That is to say that if we multiply J(t) by the instantaneous lateral root area ($2\pi s_o \ell(t)$), we get the instantaneous amount of nutrients per unit of time that the root takes; integrating this versus time, we get the proposed formula.

Thus, the goal of this paper is to evaluate the accuracy of the three formulas used in the last decades to compute the cumulative nutrient uptake by roots. Moreover, once the most suitable formula is obtained we show that this is the most appropriate formula for estimating the average simulated influx as a parameter to assess when a prediction of cumulative uptake is good or poor.

Ananalytical mass balance and the cumulative nutrient uptake formulas

In order to verify which of the formulas, Eq. (1), Eq. (2) or Eq. (3) (or its equivalent simplified expression given by (4), is more adequate, an analytical mass balance is performed according to the following procedure: if we subdivide the integration interval (t_i, t_f) from t_i until an intermediate time t and from this time t until the final time t_f, then the mentioned formulas must satisfy the mass balance when the cumulative nutrient uptake U verifies the following equality:

$$U(t_i, t_f) = U(t_i, t) + U(t, t_f), \quad \text{for all} \quad t_i < t < t_f \tag{5}$$

From here onward, we denote $U(t_i, t) + U(t, t_f)$ as SUM CUMULATIVE UPTAKE. Now, we develop our study in the following three cases:

(I) First, we analyze the Claassen and Barber formula (Eq. 1). In order to make this study easier, we simplify the referred formula by integration in parts:

$$U_{CB} = 2\pi s_o \left[\ell(t_i)\int_{t_i}^{t_f} J(s)ds + \int_{t_i}^{t_f} \underbrace{\left[\int_{t_i}^{\tau} J(s)ds + \right]}_{f(\tau)} \dot{\ell}(\tau)d\tau \right]$$

$$= 2\pi s_o \left[\ell(t_i)\int_{t_i}^{t_f} J(s)ds + f(\tau)\ell(\tau) \mid_{\tau=t_i}^{\tau=t_f} - \int_{t_i}^{t_f} \underbrace{f'(\tau)}_{J(\tau)}\ell(\tau)d\tau \right]$$

$$= 2\pi s_o \left[\ell(t_i)\int_{t_i}^{t_f} J(s)ds + f(t_f)\ell(t_f) - \underbrace{f(t_i)}_{=0}\ell(t_i) - \int_{t_i}^{t_f} J(\tau)\ell(\tau)d\tau \right]$$

$$= 2\pi s_o \left[\ell(t_i)\int_{t_i}^{t_f} J(s)ds + \ell(t_f)\int_{t_i}^{t_f} J(s)ds - \int_{t_i}^{t_f} J(\tau)\ell(\tau)d\tau \right]$$

$$= 2\pi s_o \int_{t_i}^{t_f} [\ell(t_i) + \ell(t_f) - \ell(\tau)] J(\tau)d\tau \tag{6}$$

Now, in order to decide if U_{CB} verifies Eq. (5), we compute

$$\begin{aligned}
&\frac{U_{CBS}(t_i,t) + U_{CBS}(t,t_f) - U_{CBS}(t_i,t_f)}{2\pi s_o} \\
&= \int_{t_i}^{t}[\ell(t_i) + \ell(t) - \ell(\tau)]J(\tau)d\tau + \int_{t}^{t_f}[\ell(t) + \ell(t_f) - \ell(\tau)]J(\tau)d\tau \\
&\quad - \int_{t_i}^{t_f}[\ell(t_i) + \ell(t_f) - \ell(\tau)]J(\tau)d\tau \\
&= [\ell(t_i) + \ell(t)]\int_{t_i}^{t} J(\tau)d\tau - \int_{t_i}^{t} J(\tau)\ell(\tau)d\tau + [\ell(t) + \ell(t_f)]\int_{t}^{t_f} J(\tau)d\tau \\
&\quad - \int_{t}^{t_f} J(\tau)\ell(\tau)d\tau - [\ell(t_i) + \ell(t_f)]\int_{t_i}^{t_f} J(\tau)d\tau + \int_{t_i}^{t_f f} J(\tau)\ell(\tau)d\tau \\
&= [\ell(t) - \ell(t_f)]\int_{t_i}^{t} J(\tau)d\tau + [\ell(t) - \ell(t_i)]\int_{t}^{t_f} J(\tau)d\tau \\
&= \ell(t)\int_{t_i}^{t} J(\tau)d\tau - \ell(t_f)\int_{t_i}^{t} J(\tau)d\tau - \ell(t_i)\int_{t}^{t_f} J(\tau)d\tau \\
&= [\ell(t) - \ell(t_i)]\int_{t}^{t_f} J(\tau)d\tau - [\ell(t_f) - \ell(t)]\int_{t_i}^{t} J(\tau)d\tau,
\end{aligned} \tag{7}$$

that is

$$U_{CB}(t_i,t) + U_{CB}(t,t_f) - U_{CB}(t_i,t_f) = 2\pi s_o \left\{ [\ell(t) - \ell(t_i)]\int_{t}^{t_f} J(\tau)d\tau - [\ell(t_f) - \ell(t)]\int_{t_i}^{t} J(\tau)d\tau \right\}, \tag{8}$$

and this is, in general, non-null.

In the particular case that the influx is constant, i.e. $J(\tau) = J$ in the interval (t_i, t_f), the last expression (8) reduces to

$$\begin{aligned} & U_{CB}(t_i,t) + U_{CB}(t,t_f) - U_{CB}(t_i,t_f) \\ & \quad = 2\pi s_0 J\left\{[\ell(t)-\ell(t_i)](t_f-t) - [\ell(t_f)-\ell(t)](t-t_i)^{'^{i}}\right\} \\ & \quad = 2\pi s_0 J\{\ell(t)(t_f-t_i) - \ell(t_i)(t_f-t) - \ell(t_f)(t-t_i)\}, \end{aligned} \tag{9}$$

and this is, in general, non-null. Moreover, if we define the function

$$g(t) = \ell(t)(t_f - t_i) - \ell(t_i)(t_f - t) - \ell(t_f)(t - t_i) \text{ in the interval } (t_i, t_f),$$

we can see immediately that the derivative of g(t) is given by $\dot{g}(t) = \dot{\ell}(t)(t_f - t_i) + \ell(t_i) - \ell(t_f)$,and therefore

$\dot{g}(t) = 0$ if and only if $\dot{\ell}(t) = \frac{\ell(t_f)-\ell(t_i)}{t_f - t_i} = \text{Const.}$ in the interval (t_i, t_f),

that is, the law of root growth is linear, and then the function $g(t) = g_0 = \text{Const.}$ in the interval (t_i, t_f), and therefore the expression (9) reduces to

$$U_{CB}(t_i,t) + U_{CB}(t,t_f) - U_{CB}(t_i,t_f) = 2\pi s_0 J g_0 = \text{Constant in the interval } (t_i, t_f).$$

For this reason, for any law of root growth, different to the linear case, the expression (9) is not null.

In the particular case that the influx is constant, i.e. $J(\tau) = J$ in the interval (t_i, t_f), and the law of root growth is linear, i.e. $\ell(t) = \ell(t_i) + k(t - t_i)$ in the interval (t_i, t_f), then the expression (9) reduces to

$$\begin{aligned} & U_{CB}(t_i,t) + U_{CB}(t,t_f) - U_{CB}(t_i,t_f) \\ & \quad = 2\pi s_0 J\{[\ell(t_i)+k(t-t_i)](t_f-t_i) - \ell(t_i)(t_f-t) - [\ell(t_i)+k(t_f-t_i)](t-t_i)\} \\ & \quad = 2\pi s_0 J\{\ell(t_i)(t_f-t_i) + k(t-t_i)(t_f-t_i) - \ell(t_i)(t_f-t) - \ell(t_i)(t-t_i) - k(t_f-t_i)(t-t_i)\} = 0. \end{aligned} \tag{10}$$

Thus, we have proved analytically that, for the Claassen and Barber formula (1), the condition (5) is not satisfied, in general, except when the influx J is constant and simultaneously the length of root grows linearly with the time.

(II) Similarly, for the Cushman formula (2), we can simplify the original expression to

$$\begin{aligned} U_C &= 2\pi s_o\left[\ell(t_i)\int_{t_i}^{t_f} J(s)ds + \int_{t_i}^{t_f} \underbrace{\left[\int_{t_i}^{t_i+t_f-\tau} J(s)ds + \right]}_{f(\tau)} \dot{\ell}(\tau)d\tau\right] \\ &= 2\pi s_o\left[\ell(t_i)\int_{t_i}^{t_f} J(s)ds + f(\tau)\ell(\tau)\,|_{\tau=t_i}^{\tau=t_f} - \int_{t_i}^{t_f} \underbrace{f'(\tau)}_{=-J(t_i+t_f-\tau)} \ell(\tau)d\tau\right] \\ &= 2\pi s_o\left[\underbrace{\ell(t_i)\int_{t_i}^{t_f} J(s)ds \quad +}_{f(t_i)} \quad \underbrace{f(t_f)}_{=\int_{t_i}^{t_i} J(s)ds=0} \quad \ell(t_f) - \underbrace{f(t_i)}_{=0}\ell(t_i) + \int_{t_i}^{t_f} J(t_i+t_f-\tau)\ell(\tau)d\tau\right] \\ &= 2\pi s_o\int_{t_i}^{t_f} J(t_i+t_f-\tau)\ell(\tau)d\tau. \end{aligned} \tag{11}$$

Now, in order to decide if U_C verifies Eq. (5), we compute

$$\begin{aligned}\frac{U_C(t_i,T)+U_C(T,t_f)-U_C(t_i,t_f)}{2\pi s_o}\\ &=\int_{t_i}^{t} J(t_i+t-\tau)\ell(\tau)d\tau+\int_{t}^{t_f} J(t+t_f-\tau)\ell(\tau)d\tau-\int_{t_i}^{t_f} J(t_i+t_f-\tau)\ell(\tau)d\tau\\ &=\int_{t_i}^{t} J(t_i+t-\tau)\ell(\tau)d\tau+\int_{t}^{t_f} J(t+t_f-\tau)\ell(\tau)d\tau-\int_{t_i}^{t} J(t_i+t_f-\tau)\ell(\tau)d\tau-\int_{t}^{t_f} J(t_i+t_f-\tau)\ell(\tau)d\tau\\ &=\int_{t_i}^{t}[J(t_i+t-\tau)-J(t_i+t_f-\tau)]\ell(\tau)d\tau+\int_{t}^{t_f}[J(t+t_f-\tau)-J(t_i+t_f-\tau)]\ell(\tau)d\tau\end{aligned} \quad (12)$$

and this is also, in general, non-null.

In the particular case that the influx is constant, i.e. $J(\tau)=J$ in the interval (t_i, t_f), the last expression (12) vanishes because the two brackets in the previous expression are null. Therefore, when J is constant, then U_C verifies expression (5), regardless of the law of root growth.

(III) Finally, the simplified Reginato and Tarzia formula (4) and then its original version (Eq. 3) obviously always verify condition (5) because of the linearity of the integral, i.e.

$$\int_{t_i}^{t} J(t)\ell(t)d\tau+\int_{t}^{t_f} J(t)\ell(t)d\tau=\int_{t_i}^{t_f} J(t)\ell(t)d\tau,$$

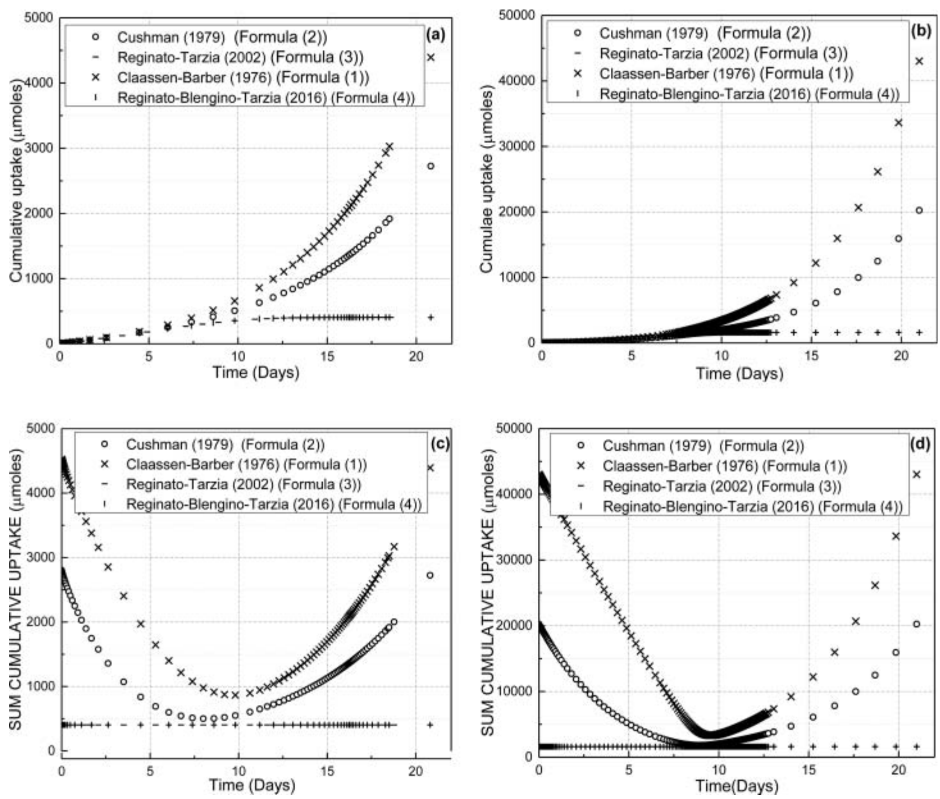

Figure 1. (a) Cumulative nutrient uptake for K uptake by maize without addition of K (low concentrations and J not constant), and (b) with addition of 250 mg kg^{-1} of K to soil (high concentrations). (c) Mass balance (Eq. 5) for four nutrient cumulative uptake formulas [Eqs.(1)–(4)] without addition of K and (d) with K addition.

and therefore we have

$$U_{RT}(t_i, t_f) = U_{RT}(t_i, t) + U_{RT}(t, t_f) \tag{13}$$

for all t in the interval (t_i, t_f).

Thus, the formula of Reginato and Tarzia always verifies the condition (5), whatever be the representative functions for the influx J(t) and the root length l(t).

Moreover, we will compare now the formulas (6), (11) and (4) through the expression (5) by means of a computational algorithm. The obtained graphs for low and high concentrations are shown in Figure 1. The data used to compute the influxes were extracted from literature for the potassium (K) uptake by maize without addition of K, and addition of 250 mg kg^{-1} of K to soil (Samal et al. 2010), and were obtained through our moving boundary model (Reginato et al. 2000) solved by the finite elements method. The same set of obtained influxes was used to obtain the cumulative uptake through the three formulas.

From Figure 1, we show that for all time t, our formula (4) always verifies the mass balance Eq. (5), while the formulas (6) and (11) do not verify it.

The use of simulated influx as an indicator to decide the rightness or wrongness of the predicted cumulative nutrient uptake

Using the correct cumulative formula (4), we can show below that the predictions based on temporal-average-simulated influx and its comparison with the influx determined experimentally by the Williams formula (1948) are only valid when the influx $J(t) = J$ is constant (for high concentrations).

If the influx $J(t) = J$ is constant, then by using the correct cumulative uptake formula (4), we obtain

$$U_{RT} = 2\pi s_o \int_{t_i}^{t_f} J(t)\ell(t)dt = 2\pi s_o J \int_{t_i}^{t_f} \ell(t)dt. \tag{14}$$

For the exponential root length growth $\ell(t) = \ell_o e^{kt}$, we get

$$U_{RT} = 2\pi s_o J \int_{t_i}^{t_f} \ell_o e^{kt} dt = \frac{2\pi s_o J}{k}\left[\ell_o e^{kt_f} - \ell_o e^{kt_i}\right] = \frac{2\pi s_o J}{k}\Delta\ell. \tag{15}$$

The last expression for U_{RT} permits us to compute the cumulative uptake from the influx J and the root length variation $\Delta\ell$. Moreover, after trivial algebraic manipulations, we obtain

$$2\pi s_o J = \frac{U_{RT}k}{\Delta\ell} = \frac{U_{RT}}{\Delta\ell}\frac{\ln(\ell(t_f)/\ell(t_i))}{t_f - t_i}. \tag{16}$$

This last expression coincides with the Williams formula. This result has been partially corroborated by an experimental work of Silberbush and Gbur (1994).

In the case that the influx J is not constant, the usually used temporal average $\bar{J}_{ta}$ of the simulated influxes is calculated by the following formula:

$$\bar{J}_{ta} = \frac{\int_{t_i}^{t_f} J(t)dt}{t_f - t_i}. \tag{17}$$

This average influx is compared with the experimental influx obtained through Williams formula, but from our previous analysis the formula (16) is consistent with the cumulative nutrient uptake formula (14) only when J is constant. Then, formula (17) is not convenient to obtain the simulated average influx when J is not constant.

In order to overcome this disadvantage, in the case that the influx J is not constant we define the temporal-weight-averaged influx $\bar{J}_{wta}$ by

$$\bar{J}_{wta} = \frac{\int_{t_i}^{t_f} J(t)\ell(t)dt}{\int_{t_i}^{t_f} \ell(t)dt}, \tag{18}$$

where $\bar{J}_{wta}$ is given in mol/cm^2 s. This temporal-weight-averaged influx is more realistic because it takes into account the temporal contribution of root length to the influx. With the expression (18) and taking into account the cumulative nutrient uptake formula (4), we deduce the Williams experimental formula (1948). Thus, replacing Eq. (4) in Eq. (18), we get

$$\bar{J}_{wta} = \frac{\int_{t_i}^{t_f} J(t)\ell(t)d\tau}{\int_{t_i}^{t_f} \ell(t)d\tau} = \frac{\Delta U/2\pi s_o}{\int_{t_i}^{t_f} \ell(t)d\tau}. \tag{19}$$

For the exponential growth case, i.e.

$$\ell(t) = \ell_o e^{k(t-t_o)},$$

we have that

$$\frac{\ell_f}{\ell_i} = \frac{e^{k(t_f - t_o)}}{e^{k(t_i - t_o)}} = e^{k(t_f - ti)}.$$

Therefore, we obtain

$$k = \frac{\ln\left(\ell_f/\ell_f\right)}{t_f - t_i}$$

and

$$\int_{t_i}^{t_f} \ell(t)dt = \ell_o \int_{t_i}^{t_f} e^{k(t-t_o)}dt = \ell_o \frac{e^{k(t_f - t_o)} - e^{k(t_i - t_o)}}{k} = \frac{\ell_f - \ell_i}{k} = \frac{(\ell_f - \ell_i)(t_f - t_i)}{\ln\left(\ell_f/\ell_i\right)}.$$

Then, replacing the last expression in Eq. (19), we get the Williams formula when the influx J is not constant for the exponential root growth law, that is

$$2\pi s_o \bar{J}_{wta} = \frac{\Delta U_{RT}}{t_f - t_i} \frac{\ln(\ell(t_f)/\ell(t_i))}{\ell_f - \ell_i}. \tag{20}$$

Similarly, for the linear growth case given by

$$\ell(t) = \ell_o + k(t - t_o),$$

we have that

$$(\ell_f - \ell_i) = \ell(t_f) - \ell(t_i) = k(t_f - t_i),$$

and therefore we obtain

$$k = \frac{(\ell_f - \ell_i)}{(t_f - t_i)}$$

and

$$\int_{t_i}^{t_f} \ell(t)d\tau = \ell_o(t_f - t_i) + k\left[\frac{(t_f^2 - t_f^2)}{2} - t_o(t_f - t_i)\right] = (t_f - t_i)\left[\ell_o + k\left(\frac{t_i + t_f}{2} - t_o\right)\right] = \frac{\ell_i + \ell_f}{2}(t_f - t_i).$$

Therefore, replacing this last expression in $\bar{J}_{wta}$, we obtain Williams formula for the linear growth case when the influx J is not constant, that is

$$2\pi s_o \bar{J}_{wta} = \frac{\Delta U_{RT}}{t_f - t_i}\frac{2}{\ell_f + \ell_i}. \qquad (21)$$

Thus, we have obtained that the cumulative uptake formula (4), the redefinition of averaged influx (18) and Williams experimental formula are well posed. We remark that Williams formula is a consequence of our definition of temporal-weight-averaged influx (Eq. 18) for all root growth law expressions. This result cannot be obtained by using the temporal-averaged influx, except in the constant influx case (for high concentrations).

Then, it is not convenient to choose the simulated temporal-averaged influxes as an indicator of a good prediction for cumulative nutrient uptake when the influx is not constant (low concentrations in the linear zone of the kinetic absorption of Michaelis–Menten), because by our formula (4) the cumulative nutrient uptake U is proportional to the influx J only when this is constant. Some papers in the literature use the simulated temporal-averaged influxes as a prediction of cumulative nutrient uptake for

Table 1. Comparison of predicted with observed Cd influx on root surface of maize, sunflower, flax and spinach on a different Cd addition [14 and 40 (+) mmol Cd/kg] to the soil. Idem for the cumulative uptake.

		Influx of Cd on root surface (10−16 mol cm^{-2} s^{-1})								
Plant	CR (10^{-3} μmol cm^{-3})	Obs.	$\bar{J}_{ta}$NST 3.0	P/O	$\bar{J}_{wta}$NST 3.0	P/O	$\bar{J}_{ta}$MB-FE	P/O	$\bar{J}_{wta}$MB-FE	P/O
Maize	0.22	0.25	2.45	9.8	2.39	9.5	1.77	7.08	0.81	3.7
Sunflower	0.38	2.12	6.11	2.9	5.74	2.7	4.74	2.23	3.29	1.5
Flax	1.19	3.54	24.4	6.9	19.9	5.6	16.6	4.69	10.7	3.0
Spinach	0.48	7.55	12.0	1.6	10.6	1.4	10.5	1.39	9.78	1.3
Maize+	0.74	1.64	7.73	4.7	7.2	4.4	5.35	3.26	1.9	1.2
Sunflower+	1.80	5.56	25.9	4.7	24.2	4.4	18.5	3.33	10.2	1.8
Flax+	4.59	10.98	82.2	7.5	73.8	6.7	61.9	5.63	44.8	4.0
Spinach+	3.07	42.11	75.0	1.8	69.8	1.7	71.2	1.69	61.1	1.4
Averaged P/O				4.98		4.77		3.66		2.24
Pearson coefficientR^2				0.737		0.754		0.836		0.894

C_R: Soil solution concentration, P/O: Predicted/Observed, Obs.: Observed, NST 3.0: Barber–Cushman model - Finite Differences, MB-FE: Moving boundary model - Finite Elements.

Table 2. Comparison of predicted with observed cumulative uptake of Cd by maize, sunflower, flax and spinach on a different Cd addition (14 and 40 μmol Cd/kg) to the soil.

Plant	CR (10^{-3} μmol cm^{-3})	Cd cumulative uptake (μmol)						
		U#Obs.	UNST 3.0	P/O	U*NST 3.0	P/O	UMB-FE	P/O
Maize	0.22	3.25	32.3	9.95	29.65	9.13	10.5	3.23
Sunflower	0.38	1.36	18.6	13.6	17.35	12.73	9.89	7.26
Flax	1.19	1.42	24.7	17.4	20.29	14.28	10.29	7.24
Spinach	0.48	3.67	5.55	1.51	5.14	1,4	4.72	1.28
Maize+	0.74	10.06	82.8	8.23	75.19	7.47	22.73	2.26
Sunflower+	1.80	8.18	83.5	10.2	77.28	9.44	32.42	3.96
Flax+	4.59	7.62	60.6	7.9	54.81	7.19	33.18	4.35
Spinach+	3.07	11.76	20.40	1.73	19.48	1.65	16.91	1.44
Averaged P/O				8.81		8.08		3.87
Pearson coefficient R^2				0.54		0.554		0.637

U_{CB} NST 3.0: Estimated with formula (1), U_{CB} NST 3.0 *: Estimated with correct formula (4).
U_{RT} MB-FE: Estimated with correct formula (4), $U^{\#}_{Obs}$: Estimated from the observed influx (by using the Williaḿs formula).

low concentrations (Stritsis, Steingrobe, and Claassen2014; Samal et al. 2010; Singh, Bhadoria, and Rakshit 2003). In order to establish the differences between the results obtained for the predicted influx by using the NST 3.0 program (Claassen and Steingrobe 1999) and our moving boundary model (MB-FE) (Reginato et al. 2000) through the temporal-averaged influx and the temporal-weight-averaged influx formula, we perform simulations with data extracted from literature. Thus, Table 1 shows the comparison among the temporal-averaged influx, the temporal-weight-averaged influx and the experimental influx obtained by the Williams formula with influxes data set obtained by Stritsis, Steingrobe, and Claassen (2014) and our moving boundary model for cadmium (Cd) uptake to different levels of Cd addition to the soil (14 and 40 μmol Cd/kg) for various crops during 43 days. The influxes set data obtained from Stritsis, Steingrobe, and Claassen (2014) are predicted by the Barber–Cushman model, which is solved numerically using the Crank–Nicholson and Newton–Ralphson techniques through the NST 3.0 software. The influxes set data predicted by our moving boundary model are obtained by using finite elements techniques (MB-FE).

The obtained results show that the averaged influxes $\bar{J}_{ta}$ and $\bar{J}_{wta}$(temporal-averaged influx and the temporal-weight-averaged influx) differ very little when these averages are obtained by using the set data of influxes provided by the NST 3.0 program (averaged P/O of 4.88 and 4.77, respectively, and, Pearson correlation coefficients of 0.737 and 0.754). Instead, when the data of influxes obtained by our model solved by finite elements technique are used, a very different result is provided (averaged P/O of 3.66 and 2.24, respectively, and, Pearson coefficients of 0.836 and 0.894), which represents an improvement of 13 and 18%, respectively, in the Pearson coefficients. Resuming, NST 3.0 overpredicts influxes (by using $\bar{J}_{wta}$) by approximately five times the measured influx, while our model MB-FE overpredicts influxes (by using $\bar{J}_{wta}$) by approximately two times the measured influx.

Table 2 show the comparison among the cumulative uptake predicted through the experimental influx obtained by the Williams formula, the cumulative uptake predicted by the original NST 3.0 program and the cumulative uptake predicted by the NST 3.0 program by using the correct formula (4) with influxes data set obtained for Cd uptake to low concentrations by various crops during 43 days (Stritsis, Steingrobe, and Claassen 2014). Also, the cumulative uptake predicted by our moving boundary model with influxes data set obtained by finite elements technique (MB-FE) by using the correct formula (4) is included in Table 2.

The obtained results show that the cumulative uptake predicted by the original NST 3.0 program and cumulative uptake predicted through the NST 3.0 program by using the correct formula (4) differ very little when are obtained by using the set data of influxes provided by the NST 3.0 program (averaged P/O of 8.81 and 8.08, respectively, and Pearson correlation coefficients of 0.54 and 0.554). Instead, when the data of influxes obtained by our model solved by finite elements technique are used to compute the cumulative uptake, a very different result is provided (averaged P/O of 3.87, and a Pearson coefficients of 0.637), which represents an improvement of 15% in the Pearson coefficient. Resuming, NST 3.0

overpredicts cumulative uptake by approximately eight times the measured cumulative uptake, while our model MB-FE overpredicts cumulative uptake by approximately four times the measured cumulative uptake.

Conclusions

The obtained results show that the Claassen–Barber and Cushman cumulative nutrient uptake formulas do not satisfy, in general, the mass balance condition (5). The Claassen–Barber formula (1) only verifies the mass balance when the influx is constant (high concentrations) and the root grows linearly. The Cushman formula (2) verifies the mass balance when the influx is constant, regardless of the law of growth. The Reginato and Tarzia formula (3) and its simplified version (4) are formulas that verify always the mass balance whatever be the representative functions for the influx and the law of root growth. Moreover, it was proved that in the case of Cd uptake when the influx is not constant, better predictions are obtained when the temporal-weight-averaged influx $\bar{J}_{wta}$is used instead of the temporal-averaged influx $\bar{J}_{ta}$(Table 1). Comparing Tables 1 and 2, we can conclude the Cd uptake and predictions of the influx on root surface in the considered case, but in case of using a more precise method (finite elements), the Cd uptake and predictions of the influx on root surface are, respectively, quadrupled and twice the observed values. Thus, predictions of cumulative nutrient uptake based on the use of the predicted averaged influx can differ significantly between them. Taking into account these results, we think that numerous papers published in the last decades based on the formulas (1) and (2) and simulated influxes for low concentrations could be reinterpreted.

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