Special Section: Model-Data Fusion in the Vadose Zone

Links Between Root Length Density Profiles and Models of the Root System Architecture

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This work aims at bridging root density profiles (i.e., root length per unit of soil volume versus soil depth) with models of the root system architecture. A sensitivity analysis was used to study the influence of root development model parameters on profile shapes and evaluate the estimation of these parameters from root density profiles.

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A lot of data is available in the literature on root length density profiles (i.e., root length per unit of soil volume versus soil depth), because they are a traditional way of representing root distribution in the field. In a complementary approach comprehensive models of the root system architecture are being developed, but the parameters required for these models are often difficult to assess in field conditions. In this paper, we bridge both approaches, empirical and comprehensive, by evaluating the capability of architectural models to simulate the observed diversity in root length distribution on the one hand and the possibility of estimating developmental parameters from root length density profiles on the other. For this purpose, we constructed a simple model with only six parameters, to represent the root system architecture. It reproduced a large diversity of root profiles comparable to observations reported in the literature and encompassing many different crops. The impact of each model parameter, as well as their interactions, on the shape of the profiles was quantified using a global sensitivity analysis. Finally, a statistical meta-model was designed and estimated to simulate the same collection of profiles without intermediate simulating the whole architecture. The meta-model allows for estimation of architectural parameters from profile shapes (inversion). Some architectural parameters could be estimated from the profiles with good accuracy, especially those quantifying the growth potential and gravitropism of individual roots, because of their specific impact on root length at a specific depth. But others (like inter-branch distance, life duration), which modify root density in a more diffuse way throughout the profile, could not be identified correctly using this method. Additional data involving specific measurements are necessary to identify these last parameters.

Abbreviations: GSA, global sensitivity analysis; IBD, inter-branch distance; IG, intensity of gravitropism; LD, life duration versus diameter; MRDB, maximal relative diameter of branch root.

Root length density profiles, that is, root length per unit of soil volume versus soil depth, are a long-standing approach for representing root distribution in the soil (Böhm, 1979), and are still commonly used (Liu et al., 2011). One reason is that root profiles inherit the usual mono-dimensional representation of the soil in terms of horizontal layers, because the soil (as well as the root system) exhibits strong vertical variations. Root profiles also stem from root observation methods, especially soil coring methods with augers, which give a direct mono-dimensional map of roots. Moreover, numerous water and nutrient uptake models use a mono-dimensional representation of root length density as the input.

Several models have been developed to directly simulate root density profiles. Among others, Gerwitz and Page (1974) and then Gale and Grigal (1987) suggested very simple statistical models to quantify and compare the distribution of various crops or biomes. Another approach was to model colonization of the soil by roots as analogous to diffusion or diffusion and convection (Page and Gerwitz, 1974; Acock and Pachepsky, 1996; de Willigen et al., 2002). The main justification for the use and development of such models is their simplicity and low number of parameters (Dupuy et al., 2010).

Nevertheless, this approach has several drawbacks. Root length density is an empirical variable which is usually obtained by averaging root lengths measured in given soil volumes collected at various depths. Its real meaning (average values and variations) is strongly dependent on the scale considered (Grabarnik et al., 1998). Root length density values become smoother with increasing scales. Moreover, a description of the integrated result of soil-root interactions is obtained, whose connection with soil and plant knowledge is not straightforward.

On the other hand, a number of authors (Pagès and Aries, 1988; Clausnitzer and Hopmans, 1994; Leitner et al., 2010) have zoomed in on the root system, and produced analysis methods and models to better understand and simulate the dynamics of the root system architecture (i.e., its shape and structure). Unfortunately, most of these models have a large number of parameters which are not easy to estimate in field conditions. Thus, they are often considered too complex for being used in crop models. Nevertheless, architectural models could help to bridge the integrated characteristics of root systems with local developmental processes occurring at the root level, as suggested by Pagès (2012). For example, these models would allow simulating root length density profiles and therefore would help linking the shape of root profiles with variations in root development.

The main aim of this paper is to reconcile both types of root system representations (root length profiles and fully fledged root system architecture) and show the possible links between these two views. This objective is justified by the large amount of data available on root profiles on one hand, and the present interest in a comprehensive view of the root system architecture on the other.

For this purpose, we (i) simulated root length profiles from a simple model of the root system architecture and evaluated how these simulations could account for the main profile variations observed in the literature; (ii) performed a global sensitivity analysis (sensu Saltelli et al., 2000) of the model parameters on the profile shape; (iii) evaluated the possibility of estimating the architectural parameters from the profile shape using a statistical meta-modeling approach to circumvent the technical problems associated to the use of stochastic architectural models.

Materials and Methods

Architectural Model

The architectural model (called the *F* model hereafter) that we used is a simple one, with only six parameters. It is a stochastic architectural model, very similar to the model of Pagès (2012), so it is only briefly outlined below, and differences are indicated.

Time is divided into daily time steps during which existing roots are virtually elongated, and new lateral axes appear by branching. The elongation rate of any root is assumed to be a linear function of its tip diameter (see Pagès, 2012), with a given slope (parameter *E*). Tip diameter is assumed to vary from one root to another within a defined range, between two threshold values (D_{min} and D_{max}). The minimal diameter (D_{min}) is the value under which no elongation is possible. The maximal value (parameter D_{max}) is the value attributed to the first root. D_{min} is deduced from D_{max} by a fixed empirical relationship ($D_{\mathrm{min}} = 0.1D_{\mathrm{max}}$).

Thus, daily elongation (L) of any root is calculated from its tip diameter (D) using the following equation:

$$\text{If } (D < D_{\mathrm{min}})\ \mathrm{L} = 0;$$

$$\text{else } (D > = D_{\mathrm{min}})\ L = E(D - D_{\mathrm{min}}) \qquad [1]$$

In this model (unlike that of Pagès, 2012), roots have a certain degree of gravitropism (parameter IG) which makes them grow downward. They die and self-prune when their age reaches a specific life expectancy and they do not longer carry any living root. The life expectancy is a linear function of the apical diameter (the slope of this linear relationship is parameter LD).

During elongation, each root was also assumed to initiate lateral primordia toward the tip, at a fixed inter-branch distance (parameter IBD). Primordia become meristems and start developing their own roots 5 d after initiation. Their initial growth direction is defined by a radial angle, measured perpendicularly to the mother root (drawn at random), and an insertion angle, measured in the common plane defined by the mother and daughter root (fixed at 80°).

The tip diameter of lateral roots (D_{l}) was calculated from the mother root diameter (D_{m}) according to the following equation with one parameter (MRDB):

$$D_{\mathrm{l}} = D_{\mathrm{m}}\ \mathrm{MRDB}e^{-u} \qquad [2]$$

u is a random number (between 0 and 3) drawn from a uniform distribution. MRDB represents the maximal diameter of the branch root relatively to its mother.

Parameter names, abbreviations, and dimensions are presented in Table 1.

Profile Calculation and Presentation

The simulated root systems were represented as sets of small segments (less than 5 mm long) and the distribution of these segments versus depth allowed the profiles to be calculated and represented either as relative length distribution versus depth (the most common way, used here for graphs), or as a collection of 9 quantiles of the depth distribution (used for statistical analyses, see below). Both presentations are formally equivalent, and have been used in the literature (e.g., Gerwitz and Page, 1974; Gale and Grigal, 1987). Figure 1 shows an example of a simulated root system together with its calculated root length profile (root length density, i.e., root length per soil volume, can be calculated from the

Table 1. Names, abbreviations, and units for model parameters.

Parameters	Abbreviation	Unit
Maximal diameter	D_{max}	mm
Slope of growth rate versus diameter	E	d^{-1}
Inter-branch distance	IBD	mm
Maximal relative diameter of branch root	MRDB	–
Intensity of gravitropism	IG	–
Life duration versus diameter	LD	$\mathrm{d\ mm}^{-1}$

number of plants per surface unit of soil to define the soil surface allocated to each plant).

Exploration of the Profiles Generated by the Architectural Model

Simulations and Global Sensitivity Analysis

We performed a global sensitivity analysis (GSA) on the developmental parameters to investigate the tuning importance of each of them on the root profiles, incorporating the whole range of their variation, as suggested by Saltelli et al. (2000). In our case, four different values, based on a large set of experimental data (see review in Pagès, 2012), were given to each parameter (Table 2). The simulated duration was 60 d.

Table 2. Values of parameters used in the sensitivity analysis.

Parameters values	1	2	3	4
Maximal diameter, Dmax	0.6	1.0	1.5	2.0
Slope of growth rate versus diameter, E	12	14	16	18
Inter-branch distance, IBD	2	4	6	8
Maximal relative diameter of branch root, MRDB	0.45	0.60	0.75	0.90
Intensity of gravitropism, IG	0.000	0.001	0.010	0.100
Life duration versus diameter, LD	120	180	300	600

Each simulated profile was represented as a series of nine depth quantiles, at nine probability levels (0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 0.98). For example, the depth quantile $q_{0.2}$ is the value for which 20% of the total root length is located above. Using nine quantiles was considered as a good compromise between information loss and redundancy. Since the model F is stochastic, three replicates were simulated for each combination of parameters and quantile values were averaged. Therefore, a total of 12,288 (3×4^6) root systems and root length profiles were simulated, resulting in a dataset of 4096 (4^6) mean profiles of 9 quantiles.

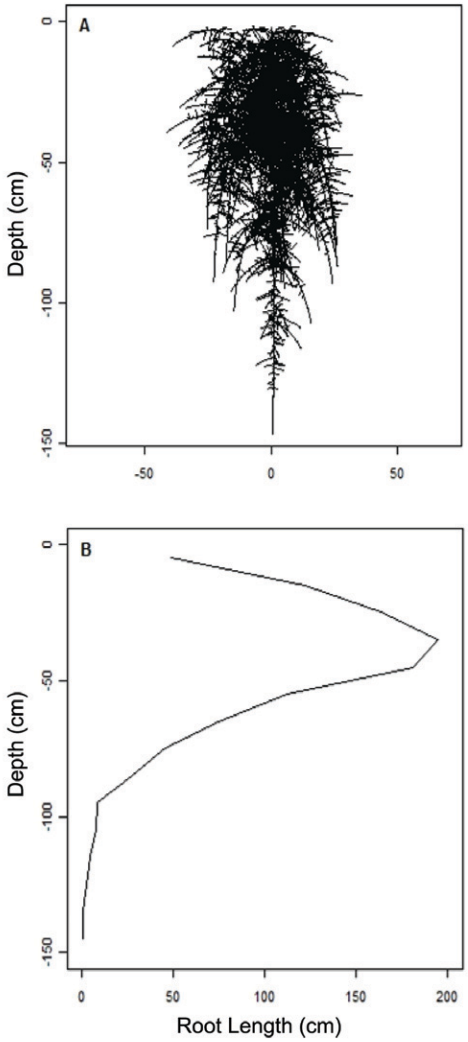

Fig. 1. Example of (A) a simulated root system with (B) the calculated root length profile.

Classification of Root Profiles

To evaluate and depict the diversity and the main variations in simulated and literature-observed root profiles, we conducted principal component analyses followed by hierarchical clustering classification, using the “FactoMineR” package in the R software (R Development Core Team, 2011; Husson et al., 2009). We used the same dataset for simulated profiles and set up a specific dataset having the same structure from observed root profiles in the literature (see Table 3 and text below).

Table 3. References from the literature reporting detailed root profiles. These references were used to build the typology presented in Fig. 3.

Source	Crops
Ahmadi et al. (2011)	field grown potatoes
Amato and Ritchie (2002)	maize
Angadi and Entz (2002)	dwarf sunflower (*Helianthus annuus* L.)
Burch (1978)	soy bean and sorghum
Camposeo and Rubino (2003)	sugarbeet
Coelho and Or (1999)	maize
Gao et al. (2010)	maize, soybean
Katayama (2000)	pigeon pea, sorghum, pearl millet, …
Kirkham et al. (1998)	maize, soybean
Lampurlanés et al. (2001)	winter barley
Lopez-Zamora et al. (2002)	peach palm
Moroke et al. (2005)	cow pea, grain sorghum, sunflower
Moroni et al. (2003)	eucalyptus
Neukirchen et al. (1999)	Miscanthus
Oikeh et al. (1999)	maize cultivars
Radersma and Ong (2004)	maize, eucalyptus, cedrella, grevilea
Sharp and Davies (1985)	maize
Zhang et al. (2004)	winter wheat
Zotarelli et al. (2009)	tomato

Analysis of Variance

We used ANOVA to study main and interaction effects of the developmental parameters on the simulated dataset. The complete balanced factorial design involving all the combinations between parameters allowed the effects to be estimated without confounding. Our ANOVA took into account the interactions until level five.

The total sum of squares SS_{tot}, representing the overall variation of quantiles was divided into components associated with different sources: main effect of each developmental parameter, and interaction effects between parameters. The effects were considered significant if the Fisher test used in the ANOVA had a p value lower than 0.05.

According to Saltelli et al. (2000), we used the main sensitivity index (I) to quantify the main effect of each parameter, and the total sensitivity index (IT) to quantify the global impact of a parameter. A difference between both indices indicates that a factor interacts with at least another one. Results are presented only for quantiles with $p = 0.2, 0.5, 0.9, 0.98$.

Meta-model Estimation and Inversion

Our goal was to find a meta-model (MF_p) that was consistent with the results of GSA and gave good prediction of the mean of quantiles. This meta-model provided a new way for calculating root profiles from the original model F. It was necessary to circumvent the technical problems associated to simulation and inversion (CPU and memory consumption, especially for big root systems, as well as algorithmic and numerical problems due to the stochastic characteristics of F during inversion). The chosen meta-model was the continuous version of the ANOVA defined as a three degree polynomial function with six input variables (developmental parameters D_{max}, E, IG, IBD, MRDB, and LD). It was interpreted as a sum of six main effects, fifteen second-order interactions and one third-order interaction (see the results). The 22 associated coefficients were estimated to minimize the sum of squares of deviations between mean quantiles and MF_p predictions. MF_p was estimated on the nine quantiles $p = 0.2,..., 0.98$. The correlations between predictions and true values are presented only for $p = 0.2, 0.5, 0.9, 0.98$.

The inversion consists in retrieving the original parameters of the F model (developmental parameters) from the nine mean quantiles, through MF_p. Since MF_p is not a linear expression of the developmental parameters, we used the Barzilai-Borwein spectral method for optimizing nonlinear objective functions subject to constraints (Varadhan and Gilbert, 2009). This method is implemented in software R (R Development Core Team, 2011).

We tested the inversion on a new sample of 100 random combinations of parameters (from Table 2), with 20 simulations per combination. Mean and standard deviation of error between inverted and true values of developmental parameters were calculated, as well as differences between the MF_p-predicted quantiles using original and estimated developmental parameters.

Results

Diversity of Simulated Root Length Profiles

Simulated root systems had highly variable total root lengths, ranging from 43 cm (minimum) to 28 km (maximum). The mean value was 658 m. Maximal rooting depth varied from 35 cm to 180 cm. With the hierarchical clustering classification, we defined five clusters, and the typical profiles for each cluster are presented in Fig. 2. This plot shows that root length profiles were also highly variable in shape. Distributions differed mainly on the superficial (versus deep) character of the distribution, and on the location of maximal density values, from close to the surface up to a depth of 70 cm. A thorough exploration showed that there were no discrete and distinct classes of rooting patterns, but all intermediate figures could be found (not shown).

Comparison between Simulated Profiles and Observed Profiles from the Literature

We used several criteria for the comparison of simulated and observed profiles: total root length (cumulated over the profile), root depth, shape of the profile, and decreasing trend with depth. A number of papers containing detailed data on root profiles (Table 3) allowed us to plot the types of profiles that are presented in Fig. 3.

Total Root Length

From some references listed in Table 3, it was possible to calculate a rough estimate of the total root length per plant (Table 4). For crop plants, total root length ranged from 700 m to 7

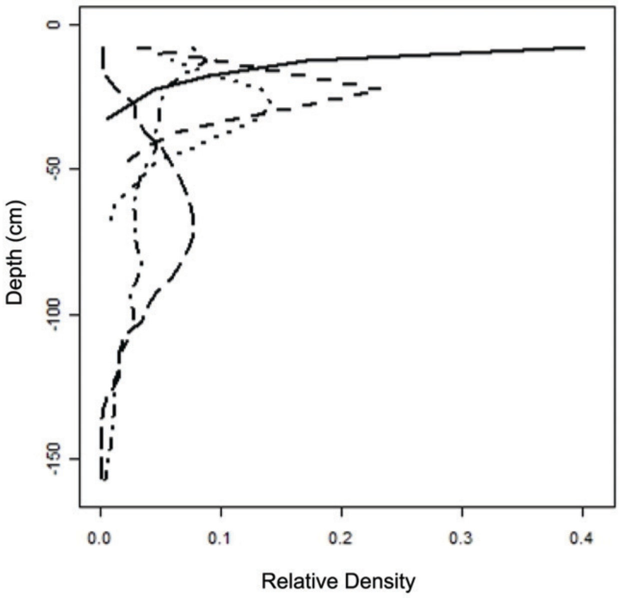

Fig. 2. Main types of simulated root length density profiles. Each line type corresponds to a different type of profile defined by hierarchical clustering classification.

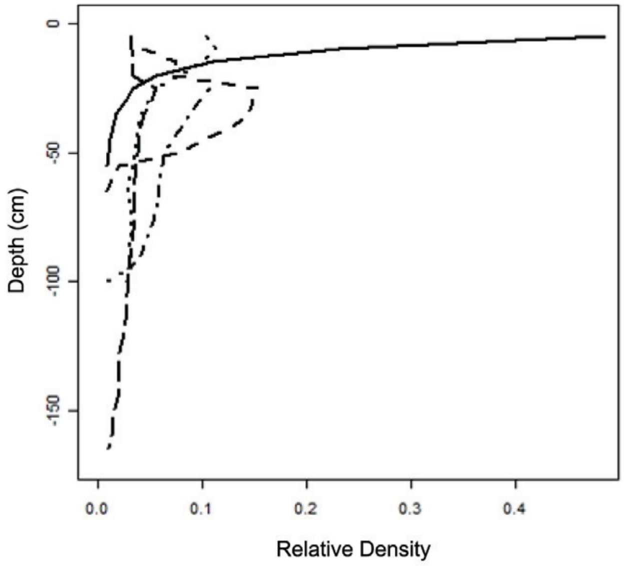

Fig. 3. Diversity of root length density profiles observed in the literature (from references listed in Table 3). Each line type corresponds to a different type of profile defined by hierarchical clustering classification.

km per plant. Lower values, as small as 31 cm were reported for small alpine plants (Pohl et al., 2011) and higher values (up to 600 km) were given for some cereals in old references (Dittmer, 1937; Pavlychenko, 1937). The model simulations covered most of this range, except for the highest values reported for some cereals. Of note, several authors mention that their length values may be underestimated due to the loss of fine roots during the excavation or washing processes.

Rooting Depth

The rooting depths observed (Table 4) ranged from approximately 30 cm to 180 cm for the set of crops, and could be as low as 15 cm for alpine plants, when small plants were growing on rocky sites. Higher values of up to several meters were found for trees and shrubs. The range observed for agricultural crops was covered by the simulated values.

Shape of the Profile

The shapes of observed profiles also showed large variations (Fig. 3). The main feature was a decreasing trend in density with depth, but this decrease could be either very sharp (superficial root systems) or rather flat (deep and evenly distributed root systems). Furthermore, it was not systematic, especially in the first 20–30 cm where the root density either increased or was stable. Interestingly, the observed types presented in Fig. 3 are comparable with the simulated types presented in Fig. 2, except the type with a maximal density near 70 cm. This shape was not encountered in the current data set.

Quantification of the Decreasing Trend

We summarized the decreasing trend by fitting the simple model of Gale and Grigal (1987). This model ($Y = 1 - \beta^d$, with Y the cumulative root fraction, i.e., the proportion of total root length to depth d in cm) quantifies the trend through the β parameter. We calculated the β values for the simulated profiles, and compared them to observed values (Table 4). Here again, the model generated a range of values consistent with those observed for various plants, except for some of the trees (Gale and Grigal, 1987) which have very deep root systems.

Table 4. Ranges of simulated and observed values for some overall characteristics.

Criterion	Simulated	Observed in literature
Total root length per plant (m)	0.43–28,000	100–7000 (in crop plants, ref. of Table 3) 0.31–170 (for alpine plants, Pohl et al. (2011)) 622,000 (Rye, Dittmer (1937)) 50000–90000 (Cereals, Pavlychenko (1937))
Root depth (cm)	35–180	30– 180 (for crop plants, ref. of Table 3) 15–70 (for alpine plants, Pohl et al. (2011))
Coefficient β of the model proposed by Gale and Grigal (1987)	0.909–0.981	0.829–0.975 (for tree species, Gale and Grigal (1987)) 0.913–0.976 (Jackson et al., 1996; Schenk, 2008)

Sensitivity Analysis of Architectural Parameters on Profile Characteristics

The ANOVA fitted the data very well, since it explained more than 94% of the variance in all cases. The most influential factor was $D_{\max}$ (IT($D_{\max}$) > 50% and I($D_{\max}$) > 40% for all quantiles) (Fig. 4). Its influence increased with the probability level p of quantile. For the higher quantile ($p = 0.98$), which approximates root depth, its role was clearly dominant (IT($D_{\max}$) close to 70%). The second important factor was IG whose main effect was decreasing with increasing probability p of the quantile (I(IG) varied from 30% to about 0%). The other factors had lower effects, although not negligible for E and RMDB for the highest quantiles. Total effect of LD was low for all quantiles (IT(LD) < 10% for all p, and was near zero when $p > 0.50$). So, LD had only a small effect on the simulated distribution of root depth. The contribution of interaction of any factor was always lower than 10%. The detailed results of the ANOVA (Table 5) showed that most second order interactions were significant, except interactions IG × LD and IBD × LD. The third order interaction $D_{\max}$ × IG × RMDB was also important for all quantiles.

Estimation of the Meta-model and Inversion

Estimation and Validation of the Meta-model

The meta-model fitted the simulated data very well and particularly the quantiles of probability greater than 0.50 (Fig. 5). The coefficients associated with the main effects were all significantly different from zero for all the analyzed quantiles. Correlations between true and fitted quantile values varied from 0.92 for p = 0.20 to 0.99 for p = 0.98. Therefore, the meta-model was considered to be a good tool to test inversion.

Tests of Inversion

The analysis of the quality of the inversion procedure was made in two steps, using a new independent sample of simulated quantiles. The values for quantiles and MF_p– predicted quantiles were very close, as shown in Table 6.

However, the correlations between the true values of the developmental parameter and inverted values by means of MF_p were: 0.87 for $D_{\max}$, 0.2 for E, 0.63 for IG, 0.38 for IBD, 0.75 for RMDB and 0.08 for LD. It means that only $D_{\max}$, IG and RMDB could be correctly estimated from the quantiles (Fig. 6). Since MF_p is close to F, this result is consistent with the sensitivity analysis of F that showed the dominant influence of these parameters.

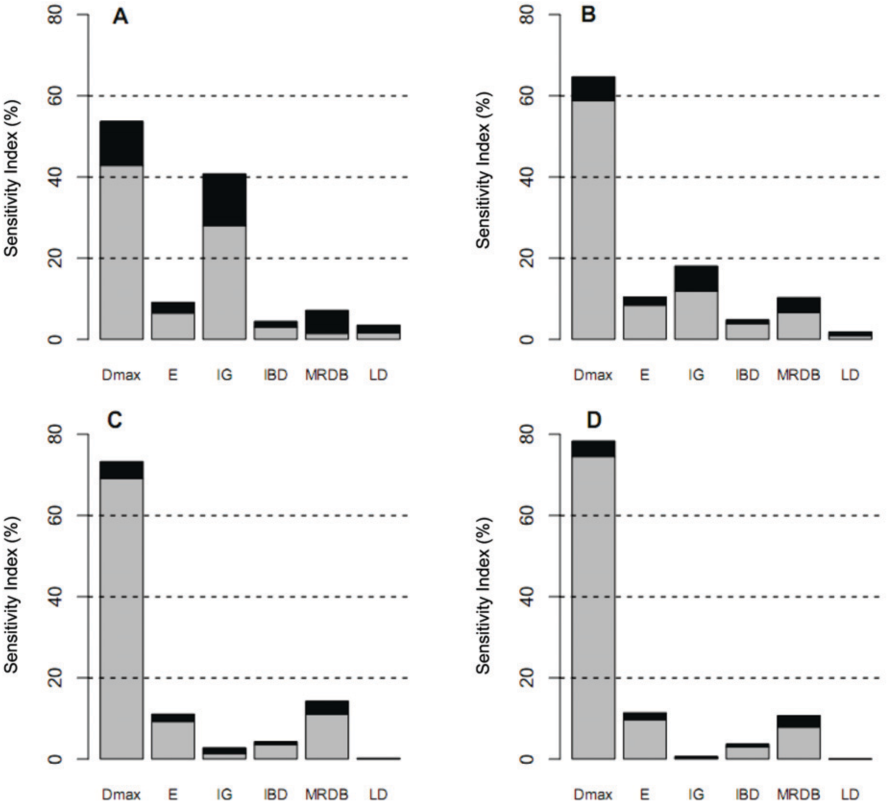

Fig. 4. Indices of sensitivity issued from the ANOVA for each parameter. Each plot is associated with a quantile: (A) $p = 0.2$; (B) $p = 0.3$; (C) $p = 0.5$; and (D) $p = 0.98$. The gray shading in bars represents the main sensitivity index in percent computed with the sum of squares of significant effects. The height of bars (gray plus black) represents the total sensitivity index in percent.

Table 5. Significant effects (p-value < 0.05) of the ANOVA of the quantiles q_p. The table gives indices of architectural parameters associated with significant effects: 1, $D_{\max}$; 2 E; 3, IG; 4, IBD; 5, RMDB; 6, LD. Interaction of parameter i and j is noted $(i \times j)$. "All" indicates that all effects are significantly different from zero. "All– $(i \times j)$" means that all effects, $(i \times j)$ excepted, are significant.

Depth quantile	Main effect	Interaction of order 2	Interaction of order 3
$q_{0.20}$	All	All– (4×6)	$(1 \times 3 \times 5)$
$q_{0.50}$	All	All– $\{(3 \times 6), (4 \times 6)\}$	$(1 \times 3 \times 5)$
$q_{0.90}$	All	All– (3×6)	$(1 \times 3 \times 5)$
$q_{0.98}$	All	All– (3×6)	$(1 \times 2 \times 5), (1 \times 3 \times 5), (1 \times 4 \times 5)$

Discussion and Conclusions

Description of Root Profiles with an Architectural Model

Using several qualitative and quantitative criteria, we have demonstrated that our architectural model does correctly simulate the global diversity of root profiles. Almost all values for the observed variables were within the range of the simulated data, with only a few exceptions. The model appeared to be well-tuned particularly for annual crop plants, about which we have the most data. However, it was run over a rather short time period and integrated a limited number of processes. Therefore, it could not simulate specific characteristics of tree or shrub root systems such as their very deep rooting depth. The simulated total root length values were also smaller than those observed for some cereals, probably because the model did not represent the crown of nodal (adventitious) roots which is specific of these plants and multiplies their total root length. Even with these limitations, the potential for this type of model is evident for representing the observed diversity, in comparison to the statistical or diffusion models that have been used (Gerwitz and Page, 1974; Gale and Grigal, 1987; Page and Gerwitz, 1974; Acock and Pachepsky, 1996; de Willigen et al., 2002). Using a large number of observed profiles, we were able to show that root density is often stable or increases in the superficial layers of soil. A monotonous decrease of root length density with depth is possible but does not hold generally (see Fig. 2 and 3).

Relative Importance of Developmental Parameters

In general, architectural models of the root system have not been designed specifically to simulate root length density profiles, but to simulate the dynamic topology and 3D geometry of root systems. Thus, the impact of the different parameters on profiles was not known and was worth studying using sensitivity analysis. We chose a global sensitivity analysis, as opposed to the "local sensitivity analysis," where the variations of each parameter are considered independently (Saltelli et al., 2000), because we were interested in both the main and interaction effects of the parameters. Analysis of variance is also a tool suited for analyzing the response of

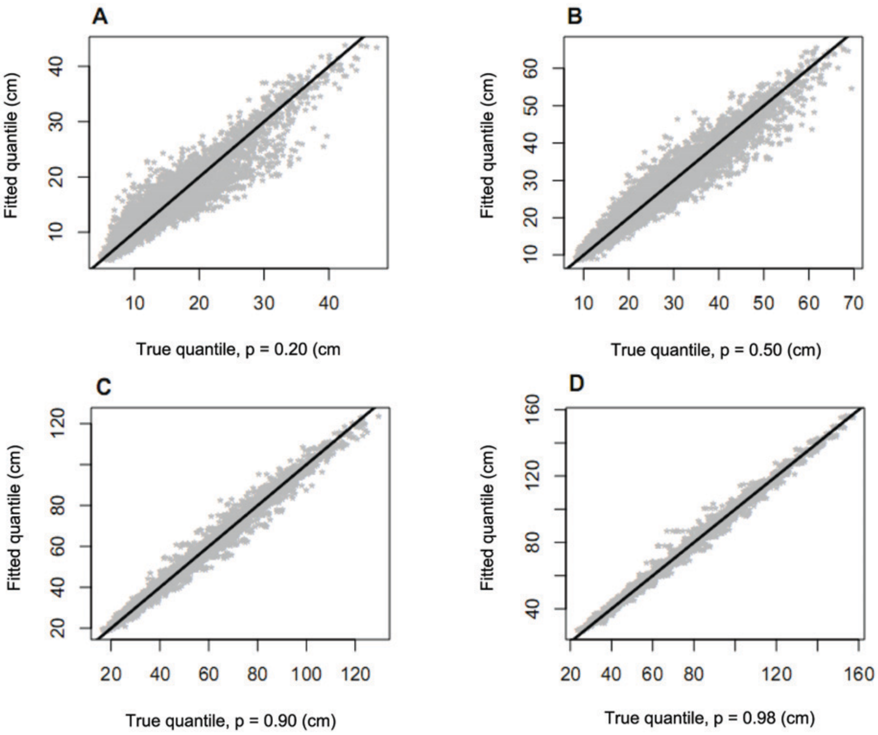

Fig. 5. Comparison of n = 4096 means of quantiles of distribution of root depths with their fitted values by the meta-model MF$_p$ (see the text). Each plot is associated with a quantile: (A) p = 0.2; (B) p = 0.3; (C) p = 0.5; and (D) p = 0.98. The line of slope 1 passing through the origin is plotted.

Table 6. Mean and standard deviation of error between true and predicted quantiles computed with the meta-model using architectural parameters obtained by inversion.

Depth quantile	Mean of error	Standard deviation of error
	cm	
$q_{0.20}$	+0.127	0.22
$q_{0.50}$	−0.037	0.18
$q_{0.90}$	+0.02	0.28
$q_{0.98}$	+0.031	0.116

profiles. Thus, we could show that the main effects of parameters were dominant, but some interactions could not be discarded.

All the parameters considered in the architectural model had a significant impact on the characteristics of root profiles. The parameters driving root elongation intensity (D_{max}, E, MRDB) and direction (IG) were dominant, when considering both main and interaction effects. Among these, parameter D_{max}, which defines the potential elongation of the roots, had a leading effect, especially for defining the rooting depth, which is a major functional variable. Gravitropism (IG) was also important since it increased particularly the lower quantiles by increasing the depth of lateral roots, especially those which appear near the base of the root system. The interactions of order 2 and 3 between D_{max}, IG, and MRDB can be interpreted as a synergistic effect between these 3 attributes, because high D_{max} and MRDB contribute to make fast-growing lateral roots, while high IG makes them grow toward the deep layers.

Although not negligible, parameters which modulate branching density (IBD and LD) had a lower impact on the profile shape, probably because their effect is diffuse throughout the root system. Their influence on total root length is much higher than that on the spatial distribution of length.

Meta-Modeling for Bridging Root System Architecture and Root Length Profiles

Starting from the results of the sensitivity analysis and the ANOVA, it was possible to design and estimate a meta-model allowing root profiles from the six developmental parameters to be directly predicted. Even though the simulation process with the architectural model and the subsequent calculations were not extremely CPU consuming, excepted for very big root systems, the link between developmental parameters and profiles was not straightforward, especially because of the stochastic character of the architectural model. It involved several simulations per combination of parameters, and then calculation of mean profiles. Meta-modeling appeared to be a convenient method to shorten this calculation chain and make it easier to invert the model (see below). Thus, the meta-model was shown to be actually a straightforward and efficient method to link developmental parameters with profile characteristics. The estimation of the meta-model coefficients (22 in our case) was facilitated by the large dataset generated by the model, and by the large number of quantiles (9) that we used to accurately characterize the profiles.

The meta-model was also used to evaluate the possibility of estimating the developmental parameters from the profile characteristics (inversion) as well as the accuracy of this estimate. Among the six parameters, three could be estimated correctly: D_{max}, IG and RMDB. They all correspond to growth characteristics. This result was not surprising, and very consistent with the ANOVA findings, which showed the dominant and independent effect of each of these three parameters on the profile responses. These three parameters act both independently and in synergy to modulate the vertical location of roots. Conversely, IBD and LD could not be identified independently from the profiles. Additional data would be necessary to evaluate these developmental characteristics. Total root length is probably a good candidate to provide complementary data, since it is often possible to calculate it from the whole profile, as we have done from data in the literature. Another possibility

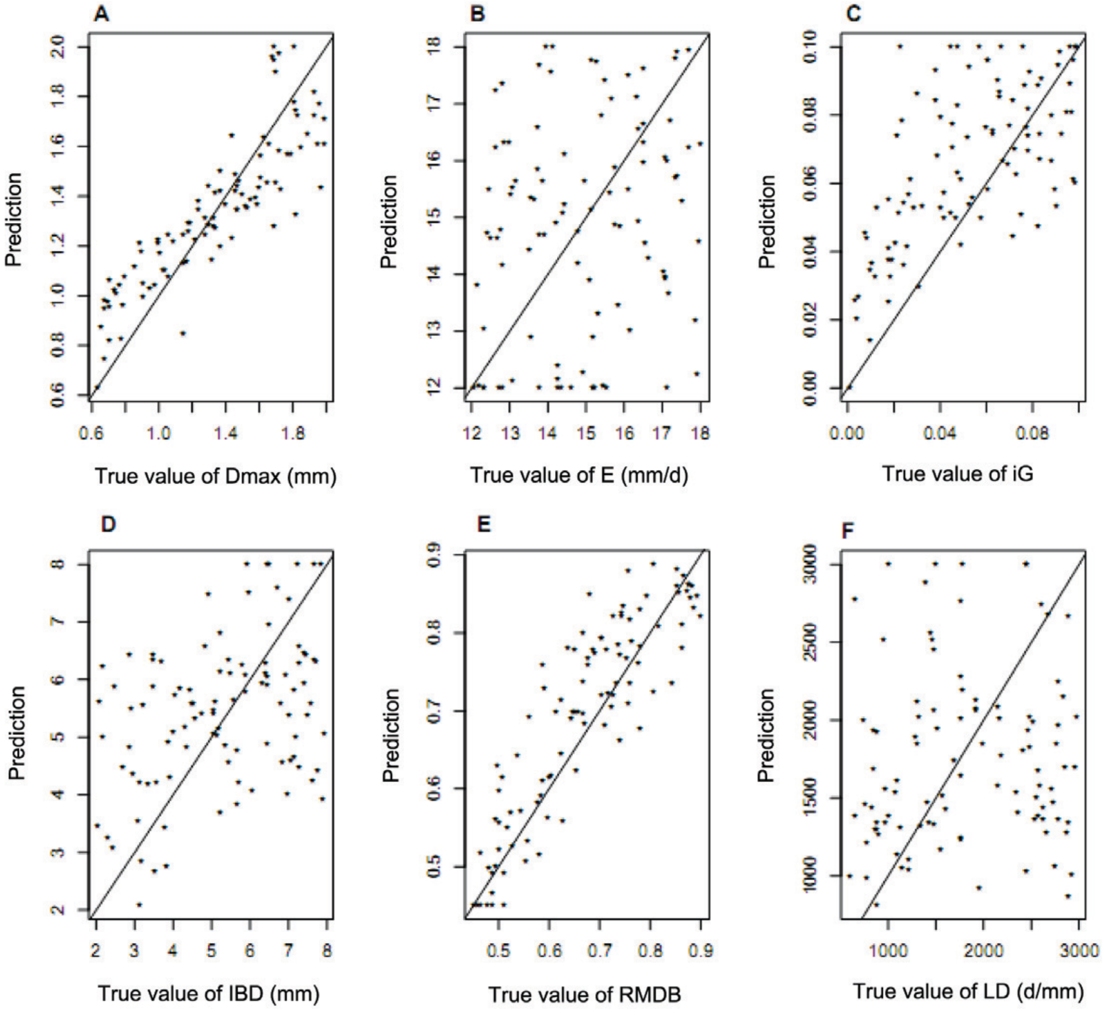

Fig. 6. Validation of inversion on a set of 100 means of quantiles different from the one used to estimate coefficients of the meta-model MF_p. Each plot compares true architectural parameter with the estimate by quantile inversion. The line of slope 1 passing through the origin is plotted.

would be to estimate more directly and independently inter-branch distance on root samples. Life expectancy of roots (LD) is probably the most difficult parameter to measure.

Beyond the particular model that we used here, which was designed simple to enable the GSA, the approach is obviously general, and can be applied to other, more sophisticated, architectural models.

Perspectives

Our findings suggest that it would be highly interesting to carry out further simulation tests aimed at assessing in greater detail which additional measurements could be the most efficient to improve estimates of architectural parameters. This question makes sense particularly for roots, because of the high cost of obtaining quality data.

Another interesting perspective would be to test other methods, such as the direct estimation of developmental parameters using the original architectural model. This may not be an easy exercise, however, because of the stochastic character of the model and the difficulty to identify independently specific parameters from root profiles. Nevertheless, we are aware that several labs are developing various methods and specific algorithms to make inversion possible even in such difficult situations.

Appendix

Global Sensitivity Analysis

In the context of the GSA, the model of the root system architecture is represented by a function F of the vector of developmental parameters ($\mathbf{X}$)

$$\mathbf{X} = (x_1, x_2, x_3, x_4, x_5, x_6)$$

with $x_1 = D_{\max}, x_2 = E, x_3 = \mathrm{IG}, x_4 = \mathrm{IBD}, x_5 = \mathrm{RMDB}, x_6 = \mathrm{LD}$. Ω is the domain of definition of F, representing the variations or uncertainty in the inputs of the model. Ω is an hypercube defined by the minimum and maximum of the admissible values of the parameters.

Let $Q_r = \left\{q_{0.2}^r, ..., q_{0.9}^r, q_{0.98}^r, r = 1, ..., R\right\}$ the overall output of the model, i.e., a set of root profiles characterized by vectors of means of depth quantiles $q_p{}^r$, R being the number of combinations of the parameters (4^6 in this case). Three random simulations (replicates) were made with the stochastic F model for each combination of parameters and the three quantile values were averaged.

We used ANOVA to study main and interaction effects of the parameters (also called factors in their discretized form). The interaction between k factors $x_{i_1}, ..., x_{i_k}$ was denoted by the k-dimensional vector of indices $u = (i_1, ..., i_k)$ associated with that interaction. For example, $u = (2, 4, 6)$ was associated with the interaction between factors x_2, x_4 and x_6. Interactions until level five were considered.

The total sum of squares $\mathrm{SS}_{\mathrm{tot}}$, variation of values $\{q_p{}^r; r = 1,..,R\}$, is a sum of components from several sources of variation: SS_i, $i = 1,..,6$, sum of squares of main effects of factor i, SS_u sum of squares of the interaction effect between factors corresponding to u belonging to the set C of combinations of indices of at most five factors, and $\mathrm{SS}_{\mathrm{res}}$, sum of squares of errors.

Thus, we have:

$$\mathrm{SS}_{\mathrm{tot}} = \sum_{r=1}^{R}\left(q_p^r - \overline{q}_p\right)^2 = \sum_{i=1}^{6}\mathrm{SS}_i + \sum_{u \in C}\mathrm{SS}_u + \mathrm{SS}_{\mathrm{res}}$$

where $\overline{q}_p = \frac{1}{R}\sum_{r=1}^{R} q_p^r$ is the total mean.

The quantity $\mathrm{SS}_{\mathrm{aov}} = \sum_{i=1}^{6}\mathrm{SS}_i + \sum_u \mathrm{SS}_u$ is associated to all the effects including factors in the ANOVA. The ratio $\tau = \mathrm{SS}_{\mathrm{aov}}/\mathrm{SS}_{\mathrm{tot}}$ quantifies the global quality of explanation of the response by factors. Effects were considered significant if the Fisher test used in the ANOVA had a p-value lower than 0.05. $\mathrm{SS}_{\mathrm{tot}}$ could be written distinguishing the sum of squares of significant and nonsignificant effects. Let SS^* the sum of squares be equal to SS if the associated effect is significant and to zero otherwise. Inversely, let SS^0 equal to SS if the associated effect is not significant and to zero otherwise. We have

$$\mathrm{SS}_{\mathrm{tot}} = \sum_i \mathrm{SS}_i^0 + \sum_i \mathrm{SS}_i^* + \sum_u \mathrm{SS}_u^0 + \sum_u \mathrm{SS}_u^* + \mathrm{SS}_{\mathrm{res}}$$

According to Saltelli et al. (2000), the main sensitivity index $I(x_i)$ of a significant main effect of factor x_i is defined by

$$Ix_i = 100\frac{\mathrm{SS}_i^*}{\mathrm{SS}_{\mathrm{aov}}}$$

The total effect of a factor x_i is quantified by $\mathrm{SS}^*_{\#i}$, sum of SS^* of significant effects taking into account at least this factor. The total sensitivity index $\mathrm{IT}(x_i)$ of factor x_i is then defined by

$$\mathrm{IT}x_i = 100\frac{\mathrm{SS}_{\#i}^*}{\mathrm{SS}_{\mathrm{aov}}}$$

The total sensitivity index quantifies the global impact of a factor on the response. A difference between main and total sensitivity indices indicates that a factor interacts with at least another one.

Meta-Model Estimation

The meta-model MF_p is the continuous version of the ANOVA defined as a 3° polynomial function with six input variables $x_1 = D_{\max}$, $x_2 = E$, $x_3 = \mathrm{IG}$, $x_4 = \mathrm{IBD}$, $x_5 = \mathrm{RMDB}$, $x_6 = \mathrm{LD}$.

$$\mathrm{MF}_p\left(X\Theta^p\right) = \mu_p + \sum_{i=1}^{6}\theta_i^p\left(x_i - \overline{x}_i\right) + \sum_{i \neq j}\theta_{i,j}^p\left(x_i - \overline{x}_i\right)\left(x_j - \overline{x}_j\right)$$
$$+ \theta_{1,3,5}^p\left(x_1 - \overline{x}_1\right)\left(x_3 - \overline{x}_3\right)\left(x_5 - \overline{x}_5\right)$$

where

$$\boldsymbol{\Theta}_p = \left(\mu_p, \theta_1^p, ..., \theta_6^p, \theta_{1,2}^p, ..., \theta_{5,6}^p, \theta_{1,3,5}^p\right)$$

is the vector of the 22 unknown coefficients and $\overline{x}_i$ the mean of variable x_i.

The meta-model was interpreted as a sum of six main effects, fifteen second-order interactions and one third-order interaction. The vector $\boldsymbol{\Theta}_p$ of coefficients was estimated to minimize the sum of squares of deviations between mean quantiles and meta-model values:

$$\sum_{r=1}^{R}\left[q_p^r - \mathrm{MF}_p\left(X, \Theta^p\right)\right]^2, p \in \{0.2, ..., 0.98\}.$$

A validation was made by comparing true values of q^r to $\mathrm{MF}_p(\mathrm{X}_r, \Theta_p)$, where θ_p was the estimated vector of coefficients. Correlation between predictions and true values were computed.

Meta-Model Inversion

The inversion consists in estimating input developmental parameters of the F model from the information of the depth quantiles. Let $\mathbf{Q} = (q_{0.2}, ..., q_{0.98})$ a vector of mean quantiles, the goal is to find the vector of architectural parameters $X^* = (x_1{}^*, ..., x_6{}^*)$ belonging to Ω and verifying $F(X^*) \sim Q^*$. We used the meta-model MF_p to minimize the deviation between Q^* and its estimation using simultaneously the nine quantiles. Let

$$\sum_{p \in \{0.2, ..., 0.98\}}\left[q_p - \mathrm{MF}_p\left(X, \Theta^p\right)\right]^2$$

be the quantity to minimize regarding to X. Let X the estimation of X^*. Since MF_p is not a linear expression of X, we used the Barzilai–Borwein spectral method for optimizing nonlinear objective functions subject to constraints (Varadhan and Gilbert, 2009).

The test of inversion was made on a new sample of size $N = 100$ of X^*. For each X^*, 20 simulations were obtained with the F model. Then, the mean values of the quantiles were computed and were associated to X^*. Mean and standard deviation of error between inverted value X of Q^* and X^* were computed. It was also verified that $\mathrm{MF}_p\left(\hat{X}^*, \Theta^p\right)$ was similar to $\mathrm{MF}_p\left(X^*, \Theta^p\right)$.

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