SimTraces a numerical simulator for predicting the accumulation of trace elements by crops

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SimTraces
A Numerical Simulator for Predicting the Accumulation of Trace Elements by Crops

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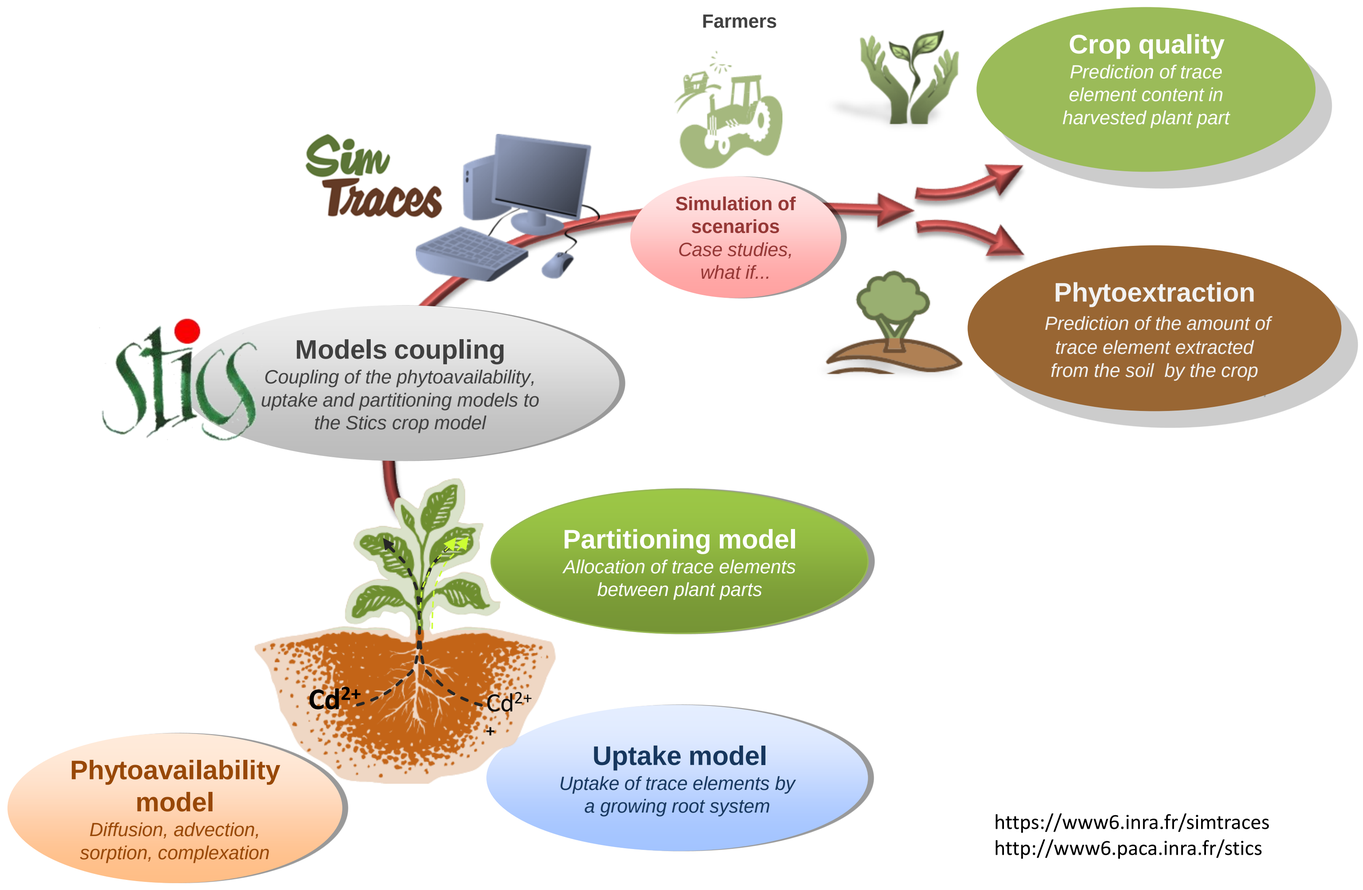
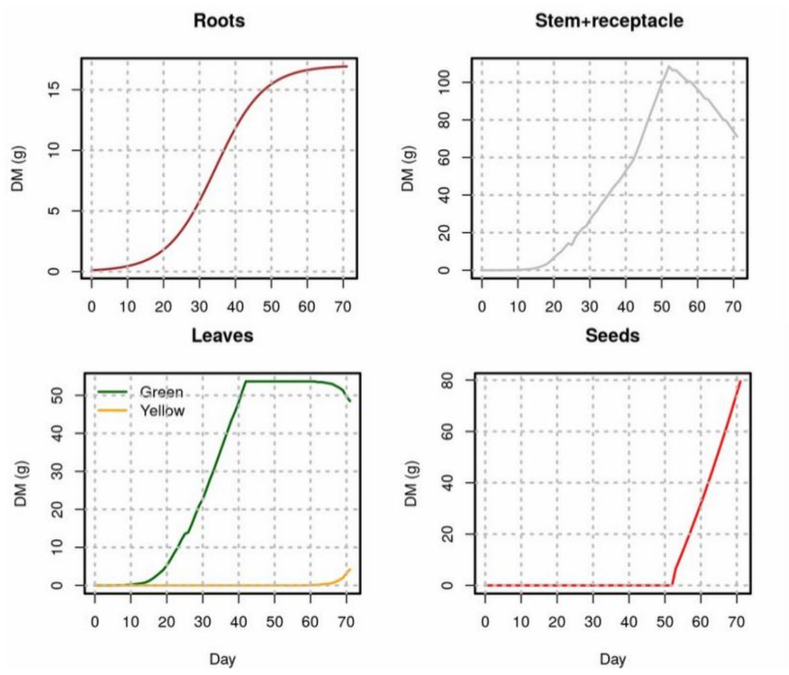
SimTraces was built with the objective of integrating all the key steps governing trace element accumulation in plant parts, taking into account the environmental conditions (climate and agricultural practices).



https://www6.inra.fr/simtraces
http://www6.paca.inra.fr/stics

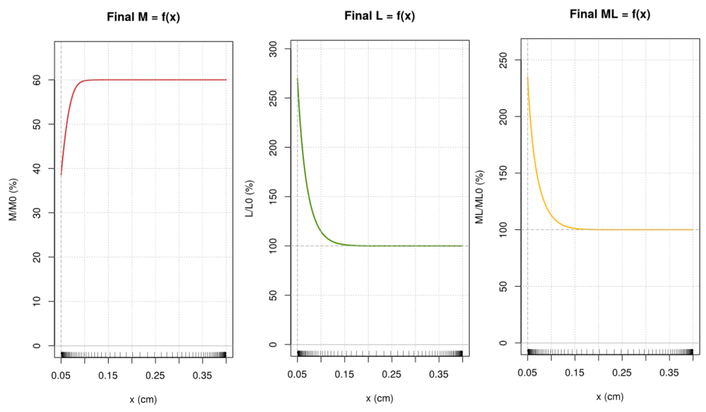
SimTraces relies on the **Stics crop model** that simulates the time course of crop growth and biomass partitioning. Three additional models have been developed and coupled with Stics.



Growth of the different plant parts of sunflower as simulated by the Stics crop model for a given set of climatic and environmental conditions.

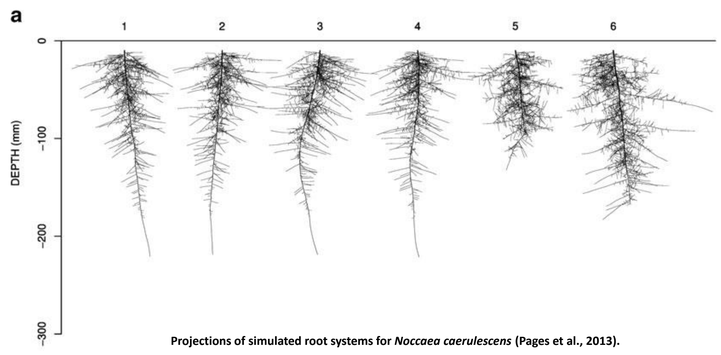
A phytoavailability model predicts the movement of the trace metal in the rhizosphere while the root absorbs it. The model considers three chemical species: the metal free ion (M), a mean organic ligand (L) and the complex between the trace element and the ligand (ML). The model accounts for the transport by diffusion and advection, for the kinetics of sorption onto the solid phase and of complexation in solution, and for the uptake by roots.

$$\theta\frac{\partial C_M}{\partial t}=\frac{1}{r}\frac{\partial}{\partial r}\left(rf\theta D_M\frac{\partial C_M}{\partial r}+r_0v_0C_M\right)+\theta\left(k_dC_{ML}-k_a^{cond}C_MC_L\right)+\left(k_{des}^{M}S_M-\theta k_{ads}^{M}C_M\right)$$
$$\theta\frac{\partial C_L}{\partial t}=\frac{1}{r}\frac{\partial}{\partial r}\left(rf\theta D_L\frac{\partial C_L}{\partial r}+r_0v_0C_L\right)+\theta\left(k_dC_{ML}-k_a^{cond}C_MC_L\right)+\left(k_{des}^{L}S_L-\theta k_{ads}^{L}C_L\right)$$
$$\theta\frac{\partial C_{ML}}{\partial t}=\frac{1}{r}\frac{\partial}{\partial r}\left(rf\theta D_{ML}\frac{\partial C_{ML}}{\partial r}+r_0v_0C_{ML}\right)+\theta\left(k_a^{cond}C_MC_L-k_dC_{ML}\right)+\left(k_{des}^{ML}S_{ML}-\theta k_{ads}^{ML}C_{ML}\right)$$
$$\frac{dS_M}{dt}=\theta k_{ads}^{M}C_M-k_{des}^{M}S_M$$
$$\frac{dS_L}{dt}=\theta k_{ads}^{L}C_L-k_{des}^{L}S_L$$
$$\frac{dS_{ML}}{dt}=\theta k_{ads}^{ML}C_{ML}-k_{des}^{ML}S_{ML}$$

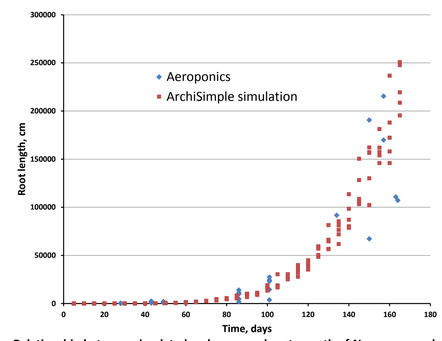


Simulation of Cd species concentrations in soil solution from root surface uptake by 1 cm root segment for 30 days in an agricultural soil.

An uptake model was built by integrating an age-dependant uptake function into a model of 3D root system architecture (ArchiSimple), which is able to simulate a great variety of root systems from few input parameters. The uptake is dynamically and spatially simulated.

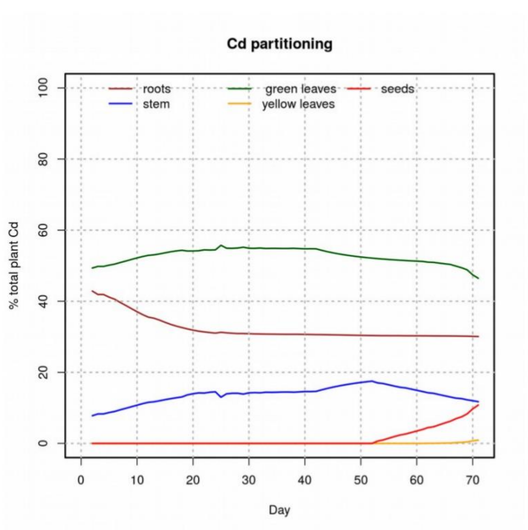


Projections of simulated root systems for *Noccaea caerulescens* (Pages et al., 2013).

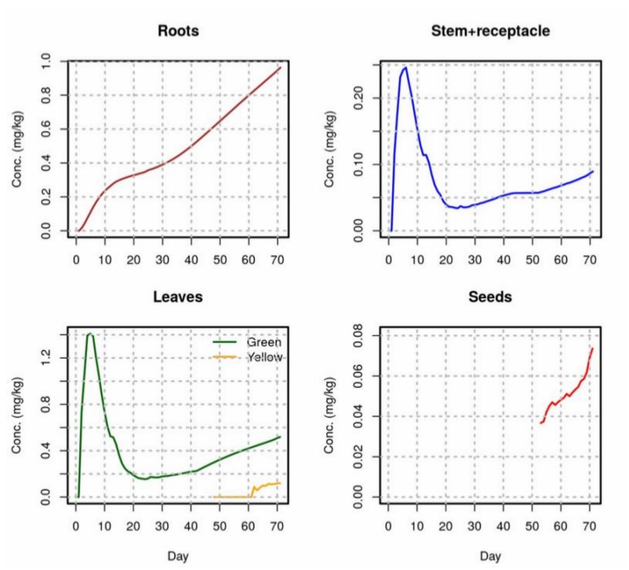


Relationship between simulated and measured root growth of *Noccaea caerulescens.*

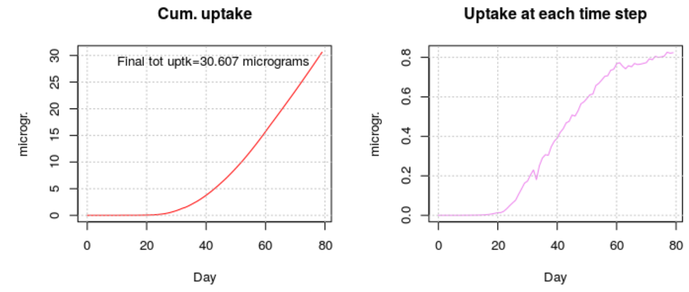
A partitioning model allows to allocate the amount of trace elements taken up at each daily time step between the different parts of the plant, the biomass of which is simulated by the Stics crop model. The partitioning is based on the transport by xylem and phloem, on exchanges between these two routes and on remobilization from senescing organs. Both the total amount of element extracted from the soil and the concentration in the plant organs are simulated along with time.



Partitioning of Cd simulated by SimTraces for sunflower from germination to maturity.



Concentrations of Cd in the different parts of sunflower as simulated by SimTraces based on the biomass dynamics simulated by the Stics crop model.



Cumulative and daily total uptake (from left to right) of Cd by a growing root system of sunflower as simulated by SimTraces.

SimTraces is an **open source** R package under construction. Besides being a **scientific tool**, it should help **agronomic expertise**, allowing agriculture and environment stakeholders to test scenarios of agricultural practices in order to optimize the quality of crop edible parts (nutrient and contaminant contents) as well as the phytoextraction of trace elements from polluted soils by dedicated crops.