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Modelling of trace metal uptake by roots taking into account complexation by exogenous organic ligands

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The context of this study is phytoextraction of soil trace metals such as Cd, Pb or Zn. Trace metal transfer from soil to plant depends on physical and chemical processes such as minerals alteration, transport, adsorption/desorption, reactions in solution and biological processes including the action of plant roots and of associated micro-flora. Complexation of metal ions by organic ligands is considered to play a role on the availability of trace metals for roots in particular in the event that synthetic ligands (EDTA, NTA, etc.) are added to the soil to increase the solubility of the contaminants. As this role is not clearly understood, we wanted to simulate it in order to quantify the effect of organic ligands on root uptake of trace metals and produce a tool which could help in optimizing the conditions of phytoextraction.We studied the effect of an aminocarboxilate ligand on the absorption of the metal ion by roots, both in hydroponic solution and in soil solution, for which we had to formalize the buffer power for the metal. We assumed that the hydrated metal ion is the only form which can be absorbed by the plants. Transport and reaction processes were modelled for a system made up of the metal M, a ligand L and the metal complex ML. The Tinker-Nye-Barber model was adapted to describe the transport of solutes M, L and ML in the soil and absorption of M by the roots. This allowed to represent the interactions between transport, chelating reactions, absorption of the solutes at the root surface, root growth with time, in order to simulate metal uptake by a whole root system.Several assumptions were tested such as i) absorption of the metal by an infinite sink and according to a Michaelis-Menten kinetics, solutes transport by diffusion with and without ii) mass flow and iii) soil buffer power for the ligand L. In hydroponic solution (without soil buffer power), ligands decreased the trace metal flux towards roots, as they reduced the concentration of hydrated metal ion. In soil, depending on the L/M ratio, the presence of metal complexes could increase the metal flux taken up by roots since the ligand desorbed the metal on soil solid phase while the complex dissociated and provided metal ions to the solution in the vicinity of the root.The model enabled to surround the conditions in which phytoextraction is thus optimized. In addition of complexation by organic ligands added to the soil, we expect to integrate complexation by roots organic exudates and by soil organic matter, as well as the competition of the metal ions with Ca2+ et H+.