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# A meta-model to predict the phytoavailability of cadmium in French agricultural soils

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## Introduction

To predict the uptake of nutrients by plant, Barber's mechanistic model simulates the behavior of only one chemical species in the soil-plant system. For metals the behavior of three species (M: free ionic  $M^{2+}$ , ML: complex of M, L: ligand, assumed unique) must be described (see Lin et al. in this session). The understanding of the results of the partial derivative equations (PDE) is difficult. Their numerical integration costs a significant time that can penalize the coupling with a more general model of transfer of metal from the soil to the crop. Steady state analytical solutions (AS) for both models were therefore developed. The outputs of PDE and AS were compared for Cd in agricultural French soils\*.

## Theory

### One species model

The Barber's model was modified to take into account the transport by diffusion and convection, the kinetics of sorption, and the Michaelis-Menten root uptake of  $Cd^{2+}$ . The PDE were as follows.

$$\left\{ \begin{array}{l} \theta \frac{\partial C_M}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r f \theta D_M \frac{\partial C_M}{\partial r} + r_0 v_0 C_M \right) + \left( k_{des}^M S_M - \theta k_{ads}^M C_M \right) \\ \frac{\partial S_M}{\partial t} = \theta k_{ads}^M C_M - k_{des}^M S_M \end{array} \right.$$

### Three species model

PDE were written for M, ML, and L, including the kinetics of complexation in solution:

$$\left\{ \begin{array}{l} \theta \frac{\partial C_M}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r f \theta D_M \frac{\partial C_M}{\partial r} + r_0 v_0 C_M \right) + \theta \left( k_d C_{ML} - k_a^{cond} C_M C_L \right) + \left( k_{des}^M S_M - \theta k_{ads}^M C_M \right) \\ \theta \frac{\partial C_L}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r f \theta D_L \frac{\partial C_L}{\partial r} + r_0 v_0 C_L \right) + \theta \left( k_d C_{ML} - k_a^{cond} C_M C_L \right) + \left( k_{des}^L S_L - \theta k_{ads}^L C_L \right) \\ \theta \frac{\partial C_{ML}}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r f \theta D_{ML} \frac{\partial C_{ML}}{\partial r} + r_0 v_0 C_{ML} \right) + \theta \left( k_a^{cond} C_M C_L - k_d C_{ML} \right) + \left( k_{des}^{ML} S_{ML} - \theta k_{ads}^{ML} C_{ML} \right) \\ \frac{\partial S_M}{\partial t} = \theta k_{ads}^M C_M - k_{des}^M S_M \\ \frac{\partial S_L}{\partial t} = \theta k_{ads}^L C_L - k_{des}^L S_L \\ \frac{\partial S_{ML}}{\partial t} = \theta k_{ads}^{ML} C_{ML} - k_{des}^{ML} S_{ML} \end{array} \right.$$

### Analytical solutions

They rely on the following assumptions:

- constant free ligand concentration
- steady state conditions
- no inter-root competition ( $\delta < r_i$ )
- cylindrical geometry

The diffusion layer thickness for a totally inert ( $\delta_{IN}$ ) or a totally labile ( $\delta_{LAB}$ ) complex is deduced from a simpler model (infinite sink, planar geometry, no convection). It increases with time:

$$\delta_{IN} \approx 0.44 \sqrt{\frac{4 f \theta D_M t}{b_M} + \frac{f D_M}{k_{ads,M}} \left( 1 - \frac{\theta}{b_M} \right)} \quad \delta_{LAB} = \delta_{IN} \sqrt{\frac{1 + \varepsilon K^*}{1 + \pi K^*}} \quad t \gg \frac{1}{4 k_{des,M}}$$

The analytical solutions of the uptake ( $U$ ) for both cases are Best's equations (van Leeuwen, 1999) differing only by the values of their  $a$ - and  $b$ -parameters:

$$U = \frac{(1+a+b)}{2b} \left( 1 - \left( 1 - \frac{4b}{(1+a+b)^2} \right)^{1/2} \right) I_{max} t$$

### One species model:

$$a_{IN} = \frac{K_m}{C_M} \left( \frac{r_0}{r_0 + \delta_{IN}} \right)^{Pe} \quad b_{IN} = \frac{I_{max}}{v_0 C_M} \left( 1 - \left( \frac{r_0}{r_0 + \delta_{IN}} \right)^{Pe} \right) \quad Pe = \frac{v_0 r_0}{f \theta D_M}$$

### Totally labile complex:

$$a_{LAB} = \frac{K_m}{C_M} \left( \frac{r_0}{r_0 + \delta_{LAB}} \right)^{\frac{1+\varepsilon K^*}{1+\varepsilon K^*} Pe} \quad b_{LAB} = \frac{I_{max}}{v_0 (1+K^*) C_M} \left( 1 - \left( \frac{r_0}{r_0 + \delta_{LAB}} \right)^{\frac{1+\varepsilon K^*}{1+\varepsilon K^*} Pe} \right)$$

### Three species model

$$\left\{ \begin{array}{l} \mu \leq \delta_{IN} \Rightarrow \mu = \sqrt{\frac{f D_M}{k_a^*}} \\ \mu > \delta_{IN} \Rightarrow \mu = \delta_{IN} \\ U = (U_{IN} - U_{LAB}) \frac{\mu}{\delta_{IN}} + U_{LAB} \end{array} \right. \quad \mu: \text{reaction layer thickness}$$

## Results

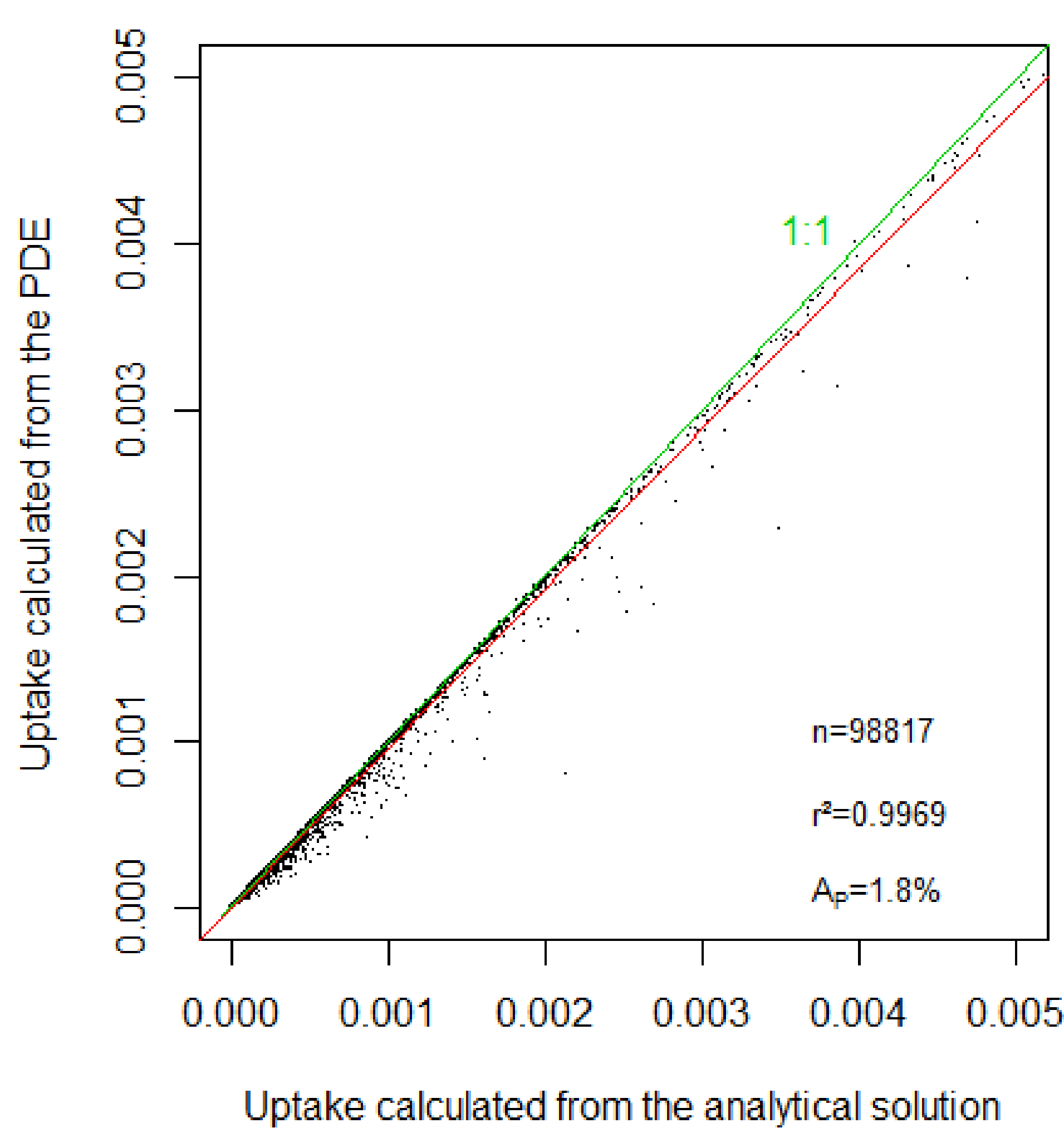


Fig. 1. One species model.

Comparison between PDE and AS outputs  
( $\mu\text{mol cm}^{-2}$  root during one month).

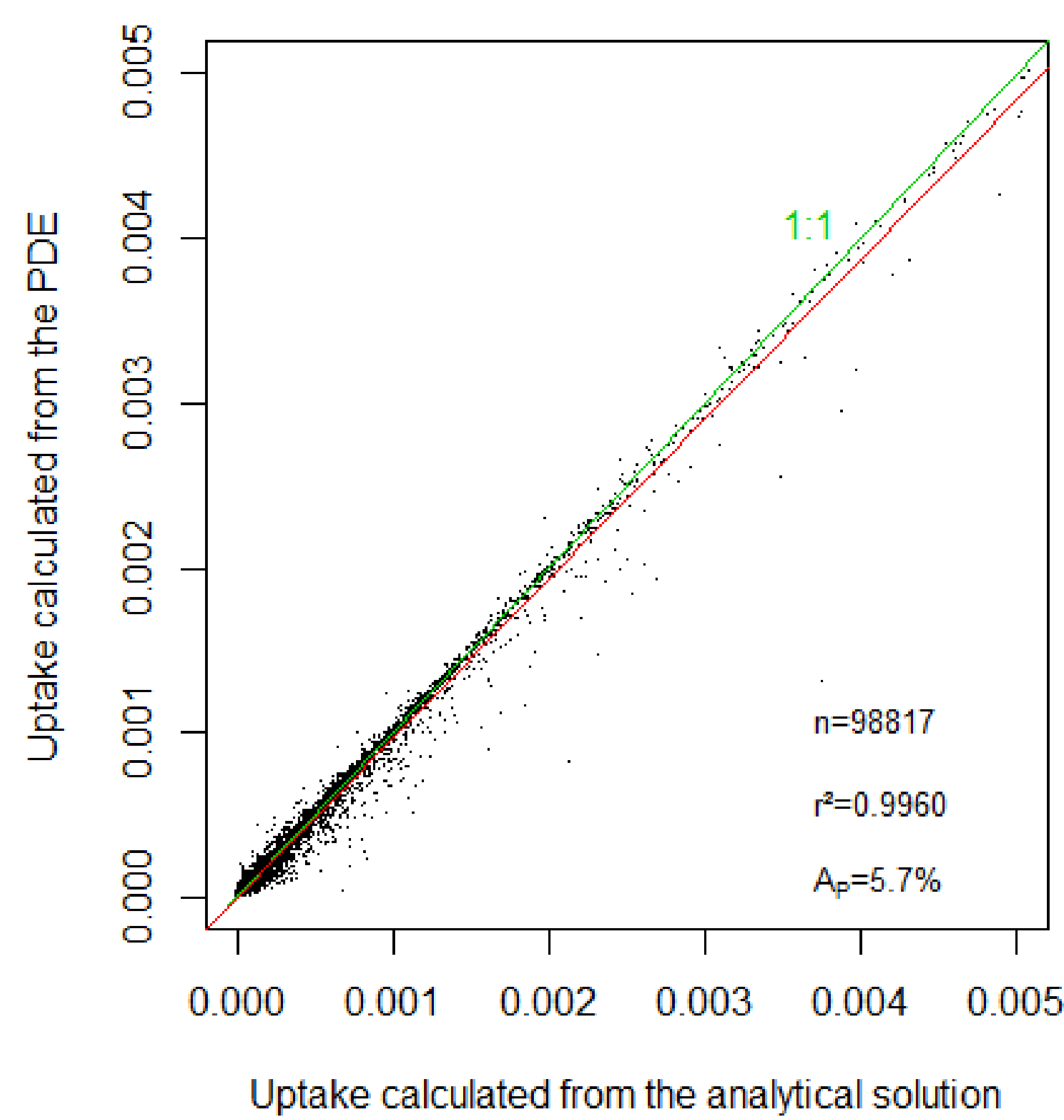


Fig. 2. Three species model.

Comparison between PDE and AS outputs  
( $\mu\text{mol cm}^{-2}$  root during one month).

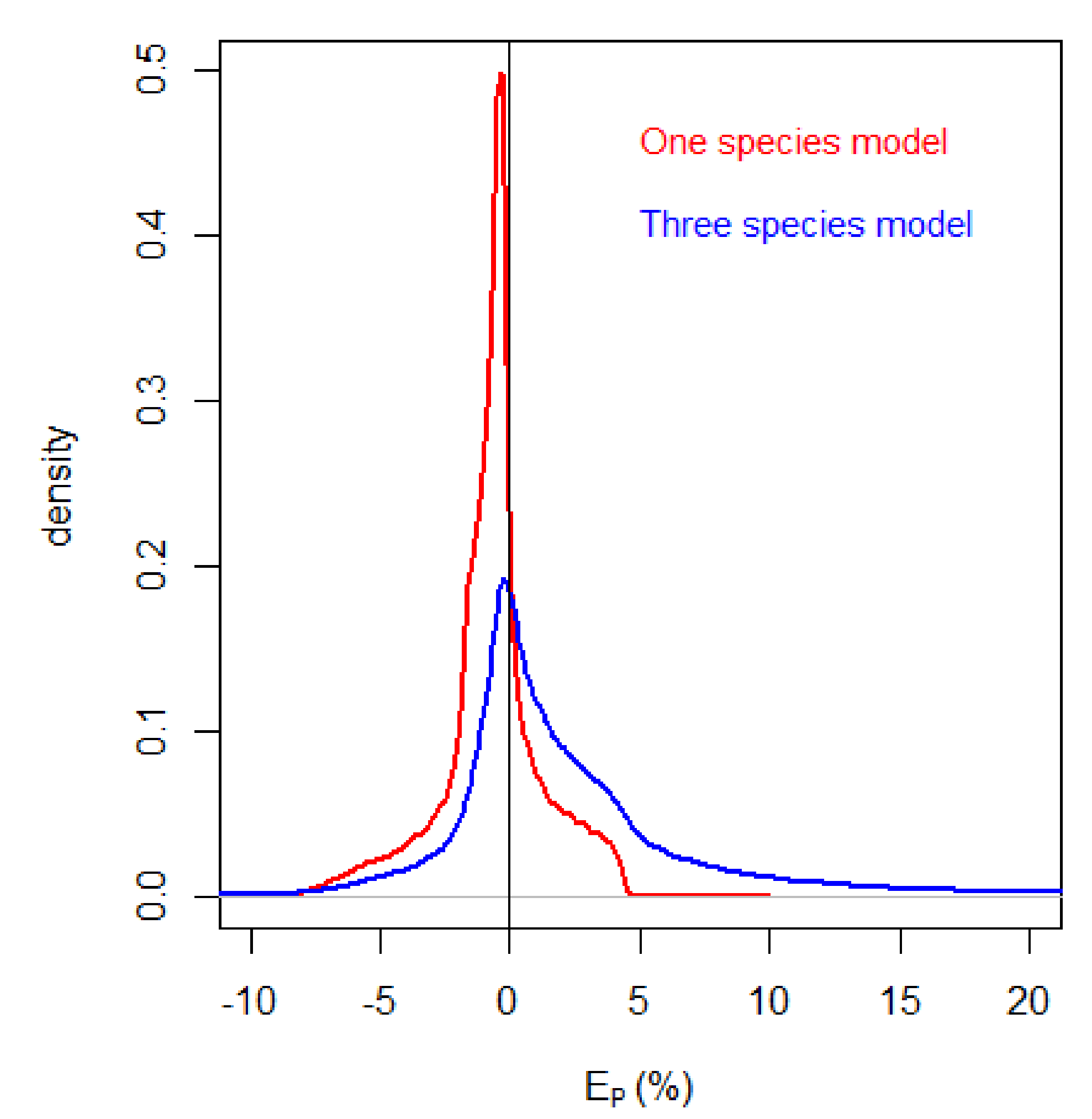


Fig. 3. Kernel density function of the relative error of prediction ( $E_p$ ) for one species model and three species model.

## Discussion and conclusion

The proposed analytical solutions constitute relatively efficient surrogates to the PDE models, even in the most realistic scenario where the lability of the complex present in solution is only partial. In this situation, the mathematical treatment stresses the importance of the reaction layer thickness ( $\mu$ ) as a crucial parameter governing the dynamics of the complex in the soil-plant system. The reaction layer is the zone close to the root where the too slow kinetics of the complexation process limits the replenishment of the metal in solution, and thus its flux toward the sink. If, during the time needed for the metal to move through the diffusion layer, the complex does not dissociate, it behaves as inert. Thus, for the complex to contribute to the uptake of the metal,  $\mu$  must be smaller than the diffusion layer thickness for a totally-inert complex ( $\delta_{IN}$ ).

## References

van Leeuwen, H.P. Metal speciation dynamics and bioavailability: inert and labile complexes. *Environ. Sci. Technol.* **1999**, *33*, 3743–3748

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\*RMQS (<http://www.gissol.fr/programme/rmq/rmq.php>)  
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