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Global Steady State Analytical Solution of Cadmium Uptake Model for Plant Roots*

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Abstract The concentration distribution of cadmium ion in soil is studied by the phytoavailability model. According to the states of the cadmium complex: fully inert, fully labile and partially labile, we establish three corresponding cadmium uptake sub-models, and derive respective global analytical solutions at steady state. In particular, when the complex is partially labile, we give the steady analytical solution of cadmium ion concentration in cylindrical geometry composed of the analytical solutions of partially labile complex and fully inert complex in planar geometry and fully inert complex in cylindrical geometry, that is, the ration approximation method. In this paper, the global analytical solutions are compared with the results of literature and numerical simulations. Therefore, the double check is realized to ensure the rationality of the analytical method. The global concentration profile of cadmium ions in the whole rhizosphere can be described by the steady state analytical solutions: the concentration of cadmium ion increases with the distance from the root surface and finally reaches the initial value; the change rate of cadmium ion concentration is the largest when the complex is fully labile; whatever the state of the complex is, cadmium ions never accumulate on the root surface. Finally, we discuss and compare the effects of moving and fixed right boundaries of the model on the results. The results show that it is more reasonable to take the fixed right boundary, and plant roots can uptake cadmium ions in a wider range.

Keywords Cadmium, complex, uptake, boundary condition

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1. Introduction

Cadmium (Cd) is one of the most toxic trace metal elements [34]. It can be absorbed through food chain and accumulated in the body, which poses a serious threat to human health [4]. The famous Itai-itai disease in Japan was caused by long-term

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consumption of rice grown in cadmium-contaminated soil [12, 24].

In the soil solution, in addition to the free Cd^{2+}, Cd also exists as complexes, which is mainly formed with soluble organic ligands [5, 6]. The concentration of Cd^{2+} on the root surface is governed by sorption, complexion reactions and transportation of Cd towards the root surface by diffusion and mass flow [1, 17, 23, 27, 32, 33]. When the ions in the soil solution mainly migrate by diffusion, the dissociation rate of complex depends on the kinetics of complexion and the concentration of free ions on the root surface [13, 14, 26, 28, 36]. The metal complexion reaction in the soil solution can be inhibited by reducing the concentration of free Cd^{2+}, so that Cd uptake by roots increases [7, 15–17, 21]. Previous studies have attempted to extend the Barbers Model to describe cadmium uptake by crops [32]. However, this model could not correctly explain why Cd complexes formed with soluble organic ligands can dissociate on the root surface [27, 29, 32]. According to the instability of the complex, Schneider distinguished three cases of the complex in the modeling, namely fully inert, fully labile and partially labile, and derived the steady analytical solutions of concentration and flux of Cd^{2+} on the root surface [28]. However, Cd is a highly-toxic metal pollutant in soil, and it is not enough to calculate and measure its concentration, flux and uptake on the root surface only. If the Cd concentration in the whole rhizosphere can be given, the pollution status of Cd in soil can be known, which is helpful for soil bio-remediation [2, 35, 37].

The nutrients uptake models by roots are governed by a convection-diffusion equation, and some solutes have complex reactions in soil such as Cd, zinc (Zn), iron (Fe) and uranium (U), and the nutrients uptake models of these solutes have the same mathematical structures, which are convection-diffusion systems. However, except that Schneider gave the analytical solution expression of Cd on the root surface, other models did not give the analytical solution. At present, researchers have given the global analytical solution of the model in planar geometry through the integral transform technique [8, 11, 18, 19, 25, 38], but only Schneider and McMurtrie have given the concentration and flux expressions on the root surface in cylindrical geometry [20, 28].

In summary, the major purposes of this paper are (1) to realize the expressions of Cd concentration in the whole rhizosphere base on the work of Schneider et al.; (2) to confirm the steady state analytical solution by the numerical solutions; (3) to adopt the fixed right boundary and compare it with the result of moving boundary.

2. The Cd uptakes models by roots

The complex behaves between two extreme situations, namely, the inert and the fully labile complexes. For the inert complex, the complexion kinetics are so slow compared to other mechanisms that the complex dissociation cannot significantly buffer the free ion concentration in the solution. For the fully labile complex, the association-dissociation kinetics are so rapid that the free ion and the complex are always at equilibrium temporally and spatially. Between these two extremes, the complex is partially labile and its contribution to the uptake is lower than the maximum contribution reached by the fully labile complex [28].

Based on the model built by Schneider et al., the situation where an organism is in contact with medium containing free ions (m), and complex metal ions (ml) is considered [28]. The interconversion between two species is governed by the association-dissociation reaction of m with the ligand l [13]