MATHEMATICAL MODEL OF PHYTOEXTRACTION FOR CONTAMINATED SOILS

by

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Submitted

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to the

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Dedicated

to

My Loving Mother.....

Resting peacefully at the Lotus Feet of God Almighty

CERTIFICATE

This is to certify that the thesis, entitled "***Mathematical Model of Phytoextraction for Contaminated Soils***", being submitted by Mr. Brijesh Kumar Yadav to the Indian Institute of Technology, Delhi for the award of Doctor of Philosophy, is a record of bonafide research work carried out by him under my supervision. The thesis work, in my opinion has reached the standard, fulfilling the requirements for the said degree. Further, I certify that this submission is Mr. Yadav's own work and that, to the best of my knowledge and belief, it contains no material previously published or written by another person which to a substantial extent has been accepted for the award of any other degree or diploma of any University or Institute, except where due acknowledgment has been made in the text.

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ABSTRACT

Phytoextraction is an eco-friendly remediation technology which uses plants for removing heavy metal contaminants from polluted soils. The effective implementation of this cost-effective emerging technology requires a conceptual insight of soil and plant processes that control the extraction of targeted contaminants from the problem area. Most of the current research deals with the plants grown on heavy metal contaminated soils and analyzed experimentally to determine their capacity to remove them from the soil. Prediction of the metal uptake by plants through mathematical modeling has received very little attention so far due to the complexity of the soil-plant-atmosphere continuum.

In this study, a mathematical model is developed to investigate the removal of a heavy metal from contaminated soil by plant root biomass. The model comprises two parts; 1) soil moisture flow and plant water uptake modeling and 2) modeling heavy metal contaminant transport and metal extraction by the plant root biomass. The soil moisture movement and uptake of soil water by roots from variably saturated soils is predicted first. The metal extraction by plant root biomass is simulated next using the observed plant-soil parameters and the moisture flow data simulated from the first part of the model.

In the first part, a non-linear macroscopic plant water uptake model that includes the impact of soil moisture availability (quantity) and soil solution salinity (quality) is

developed to predict the actual water uptake by plants and the hydraulic regime of the soil profile for different environmental conditions. The model also incorporates the spatial and temporal variation of root density distribution in addition to the dynamic root depth considerations. The governing partial differential moisture flow equation coupled with the plant water uptake function is solved numerically by the implicit finite difference method using Picard's iterative scheme.

Initially, the soil moisture flow model is tested without considering the water uptake by root term for the two test cases considering constant infiltration and a constant pressure head surface boundary condition. The results obtained are later tested with experimental data available in literature. A non-linear plant water uptake term is subsequently incorporated in the model which is then applied to five plant water uptake scenarios under different environmental conditions. A constant root depth is considered in these five scenarios. In the first three plant water uptake cases, different root distribution patterns namely: constant, linear and non-linear (decreasing with soil depth) are considered with and without soil moisture limitation. Later, a dynamic plant root water uptake mechanism is considered in the fourth application taking the non-linear root distribution pattern under optimal and soil moisture deficit conditions. The impact of soil solution salinity is not considered in these four cases. The last plant water uptake scenario is applied to a salt affected arid and semi-arid environment. Finally, the moisture flow model is applied to a corn growing field and simulated results are validated with the available field measured data in the literature. The simulated moisture content for two months of crop growing season shows reasonably good agreement with the observed data.

In the next part of the study, a mechanistic model for metal extraction by plant root biomass is developed. First, the contaminant transport equation without a metal uptake by plant term is solved numerically for a simplified case using the Crank-Nicholson finite difference scheme coupled with the Picard iteration scheme. In order to circumvent the problem of numerical smearing or oscillation, the stability requirement is achieved by satisfying the Courant and Peclet numbers. Then, A simultaneous movement of soil water and solute transport is simulated by coupling moisture flow model with the contaminant transport model. The Michaelis-Menten active uptake kinetics is used for simulating the metal extraction mechanism by the plant root biomass. Lastly, the model is applied to a hypothetical case using observed soil-plant model parameters to study phytoextraction of lead using corn plants.

CONTENTS