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Modeling of Sequential Dissipation of TNT in Phytoremediation

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Abstract

Plants may enhance the remediation of munitions at contaminated soils using various natural processes. A computer model can be used as a valuable tool for assisting phytoremediation by predicting the transport and fate of target contaminants at remediation sites. For this research, modeling of phytoremediation and bioremediation of soil contaminated with 2,4,6-trinitrotoluene (TNT) was studied. Indian mallow (Abutilion avicennae) was grown in columns packed with 126 mg TNT/kg contaminated soils for 50 days and a simulation model was developed to simulate the transport and fate of TNT and its breakdown products interacting with plant roots in a partially saturated soil. The column test showed the substantially enhanced reduction of TNT and greater soil microbial activity in Indian mallow planted soil compared to unplanted soil. The model successfully simulated the fate of TNT and by-products in phytoremediation. The results suggested that plants could provide favorable environments for reduction of TNT.

key word: phytoremediation, simulation model, 2,4,6-TNT, sequential dissipation

1. Introduction

Explosives like 2,4,6-trinitrotoluene (TNT), released to the soil and groundwater at military bases and ammunition manufacturing facilities, can lead important environmental issues due to their high toxicity and persistency (Sens et al., 1999). Plants may enhance the remediation of munitions at contaminated soils using various natural processes and provide a cost-effective alternative, especially for large volumes of contaminated soil (Voudrias and Assaf, 1996). Although plants can uptake TNT from hydroponic solution, only few % of TNT and its by-products were found in soil-plant system (Palazzo and Leggett, 1986; Thompson et al., 1998). TNT can be degraded or transformed by co-metabolism under aerobic and/or anaerobic conditions (Boopathy et al, 1994). TNT can reduce to 2-amino-4, 6-dintrotoluene (2-AMDNT) and 4-amino-2, 6-dinitrotoluene and then reduced again to diamino-nitrotoluene (DANT) and other reaction products (Harvey et al., 1990). Major pathways of TNT dissipation in soil were biodegradation and sorption (Cataldo et al., 1989). The purpose of this research was to evaluate the effectiveness of Indian mallow on TNT dissipation and to develop a simulation model that can estimate the fate and transport of TNT and its breakdown products in phytoremediation.

2. Model Development

A two-region (rhizosphere and bulk) soil model for phytoremediation (Sung et al., 2003) was modified to simulate the TNT and its breakdown products in a sequential pattern. The general form of the mass balance equation of TNT and its sequential by-products in the soil water phase of a rhizosphere and bulk soil can be expressed as;

$$\frac{\partial \theta_w C_{rhw,i}}{\partial t} = -\frac{\partial}{\partial z}\left(q_w C_{rhw,i} - D_{Hw}\frac{\partial \theta_w C_{rhw,i}}{\partial z}\right) - a_{s,i}\rho_b \left(K_{1,i}C_{rhw,i} - C_{rhs,i}\right) - \frac{\partial}{\partial t}\left(K_{bs,i}C_{rhw,i}C_{rhm}\right)$$
$$-\sigma_r K_{nrw,i}\left(K_{rw,i}C_{rhw,i} - C_{r,i}\right) - k_{m,i}C_{rhm}\left(\frac{C_{rhw,i}}{K_{w,i} + C_{rhw,i} + K_{I,i}C_{rhw,i}^{2}}\right)\left(\frac{C_{rhp}}{K_p + C_{rhp}}\right)$$
$$-U_w T_{scf,i}C_{rhw,i} + k_{m,i-1}C_{rhm}\left(\frac{C_{rhw,i-1}}{K_{rhw,i-1} + C_{rhw,i-1} + K_{I,i-1}C_{rhw,i-1}^{2}}\right)\left(\frac{C_{rhp}}{K_{rhp} + C_{rhp}}\right) + K_{wbr}\theta_w\left(C_{bw,i} - C_{rhw,i}\right) \quad (1)$$

3. Materials and Methods

TNT (Chem Service, USA) was mixed with the sandy loam soil to the initial concentration of 126 mg TNT / kg soil. This soil was 14.96% clay, 7.84% silt, and 77.2 % sand containing 8 % of organic carbons. Soil pH was 5.67. The specially designed PVC columns (10 cm in diameter and 100 cm in depth) were used for sampling of microbial activity, root properties and contaminant concentrations with depth. Uncontaminated soil was first filled up to 80 cm from the bottom and then contaminated soil was compacted upper 20 cm. After 4 days of stabilization period, Indian mallow (Abutilion avicennae), that have grown for 7 days after germination, were planted at a rate of 3 seeds per column. The experiments were conducted for 50 days and root properties, microbial activity, concentrations of TNT and its breakdown products in soil and plants were measured.

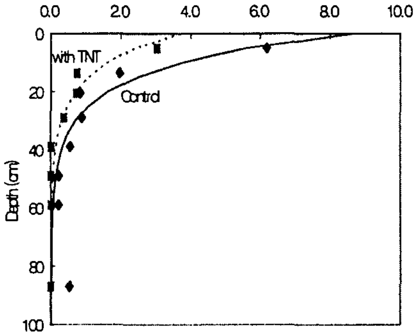

Fig. 1. Comparison between measured and simulated spatial variation of rooting density of Indian Mallow planted column at 50 day after seeding

4. Results

Figure. 1 shows the measured and simulated rooting density profiles of Indian Mallow planted column with and without TNT contamination. There was a significant reduction of total rooting mass and rooting density of Indian Mallow at TNT contaminated soil due to its toxicity.

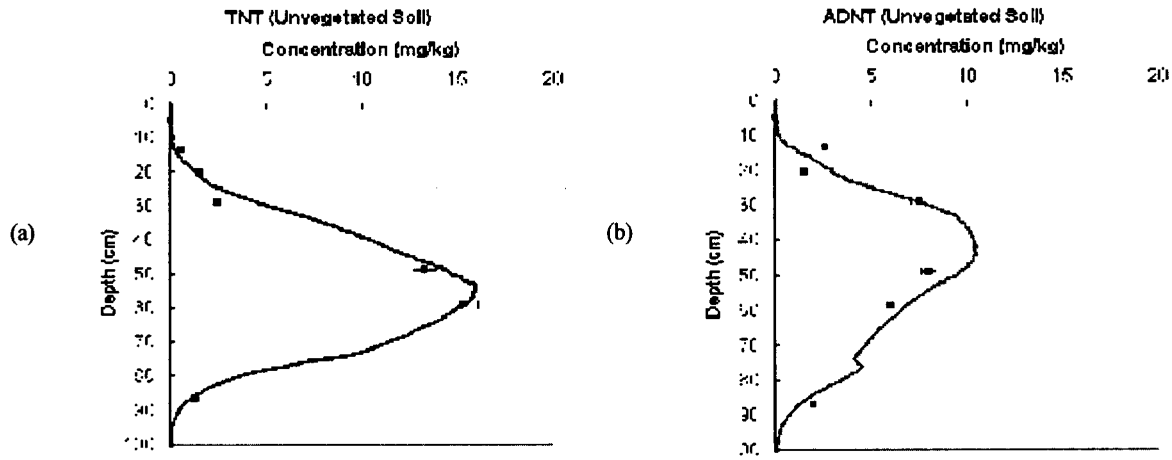

Fig. 2. Comparison of simulation results with experimental data of (a) TNT and (b) ADNT concentrations for unvegetated soil at day 50.

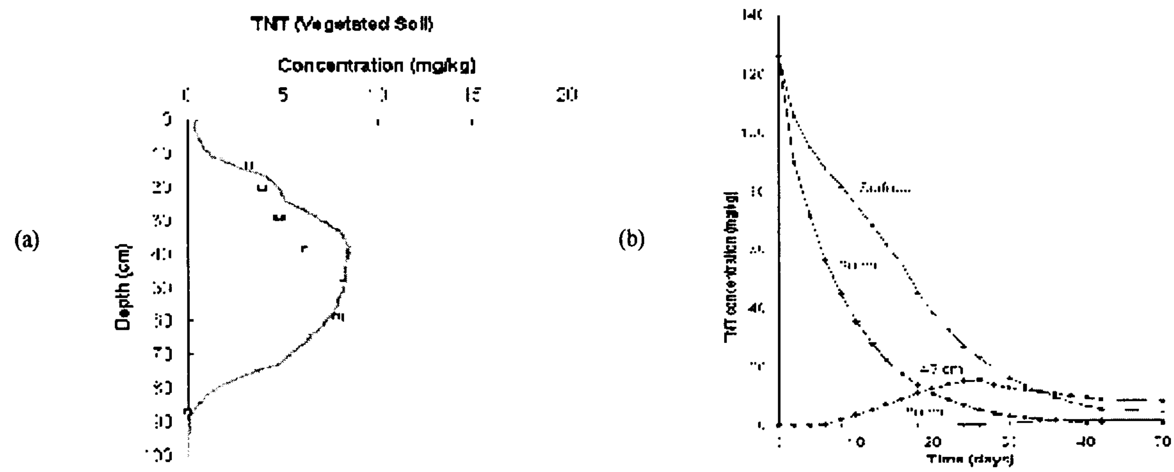

Fig. 3. (a) Comparison of simulation results with experimental data of (a) TNT in Indian Mallow planted column at day 50 and (b) temporal variation of the TNT concentration at each depth until 50 day.

Figure 2 illustrates the simulated values with experimental data of TNT and ADNT concentrations for unvegetated columns at day 50. Figure 3 shows the TNT concentration change at each depth until day 50 and model comparison with experimental data of TNT in Indian Mallow planted columns at day 50. Results indicate good correlation between simulated and experimental data with little difference. It is observed from the model simulations that the soil column planted with Indian Mallow enhanced remediation of TNT by stimulating microbial activity. The temporal and spatial fate of TNT and its breakdown products also depends on the frequency and quantity of water irrigation as well as microbial activity and the sorption properties of chemicals and medium. Migration of breakdown products from TNT and ADNT by the rapid dissipation of TNT in the Indian Mallow planted column can be retarded due to root effects.

Acknowledgments

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