A Method to Decide Diffusion Coefficient of Heavy Metals in Soil

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The great leader Comrade **Kim Jong Il** said as follows.

"Another important matter in land management is to do everything possible to improve the soil."

It is important to decide the diffusion coefficient correctly to diagnose and predict about the diffusion of heavy metals correctly in soil. There was a study to decide separately diffusion coefficient and solutions of prediction equations. [1-3] This paper it was discussed about a method to decide diffusion coefficient of heavy metals in soil.

1. Convection diffusion equation of heavy metals in soil

In soil a diffusion equation of heavy metals are as follows. [1]

$$m\frac{\theta}{\theta_s}\frac{\partial c_j}{\partial t}+\theta u\frac{\partial c_j}{\partial z}=\frac{\partial}{\partial z}\left(D_j\frac{\partial c_j}{\partial z}\right)-\frac{\partial s_j}{\partial t} \tag{1}$$

$$\frac{s_{\text{Na}}}{\sqrt{s_{\text{Pb}}}}=K_{\text{Na-Pb}}\frac{c_{\text{Na}}}{\sqrt{c_{\text{Pb}}}} \tag{2}$$

$$\frac{s_{\text{Na}}}{\sqrt{s_{\text{Cd}}}}=K_{\text{Na-Cd}}\frac{c_{\text{Na}}}{\sqrt{c_{\text{Cd}}}} \tag{3}$$

$$s_{\text{Na}}+s_{\text{Pb}}+s_{\text{Cd}}=N_0(z) \tag{4}$$

Initial condition

$$t=0\,;\begin{cases}c_j(z,\ 0)=c_{j0}(z)\\ s_j(z,\ 0)=s_{j0}(z)\end{cases} \tag{5}$$

Boundary condition

$$t>0\left\{\begin{array}{l}z=0;\quad c_j(0,t)=\varphi_j(t)\\ z=L;\quad \dfrac{\partial c_j(L,t)}{\partial z}=0\end{array}\right\} \tag{6}$$

Where $c_j(z,t)$ is a concentration of j ion in soil solution (mg/100g), $s_j(z,\ t)$ is a concentration of j ion in soil absorbing complex(mg/100g), K_{A-B} is a selectivity coefficient of ion exchange, D_j is a diffusion coefficient (m^2/d), *m* is a sponginess of soil, θ is a moisture of soil, θ_s is a saturated humidity of soil, u is a vertical travelling speed of soil moisture (m/d), t is a time scale (d) and z is a depth of soil (m).

First, let's convert all variables in Eq. (1) - (6) into dimensionless quantities.

$$\left.\begin{aligned} & p_j(\xi,\ \tau) = \frac{c_j(z,\ t) - c_{\Pi j}}{c_j^* - c_{\Pi j}} \\ & \tau = \frac{u^* t}{mL} \\ & \xi = \frac{z}{L},\ N_j(\xi,\ \tau) = \frac{s_j(z,\ t)}{N_j^*} \end{aligned}\right\} \tag{7}$$

Where c_j^*, u^* and N_j^* are characteristic coefficients and $c_{\Pi j}$ is a concentration of j ion in the irrigation water or rainwater (mg/100g).

Then, the Eq. (1) - (7) are converted as follows.

$$\frac{\theta}{\theta_s}\frac{\partial p_j}{\partial \tau} + \theta f \frac{\partial p_j}{\partial \xi} = \frac{\partial}{\partial \xi}\left(\frac{1}{p_{ej}}\frac{\partial p_j}{\partial \xi}\right) - \frac{N_j^*}{m(c_j'' - c_{\Pi j})}\frac{\partial N_j}{\partial \tau} \tag{8}$$

$$\frac{N_{\mathrm{Na}}^* N_{\mathrm{Na}}}{\sqrt{N_{\mathrm{Pb}}^* N_{\mathrm{Pb}}}} = K_{\mathrm{Na-Z}n}\frac{p_{\mathrm{Na}}(c_{\mathrm{Na}}^* - c_{\Pi\mathrm{Na}}) + c_{\Pi\mathrm{Na}}}{\sqrt{p_{\mathrm{Pb}}(c_{\mathrm{Pb}}^* - c_{\Pi\mathrm{Pb}}) + c_{\Pi\mathrm{Pb}}}} \tag{9}$$

$$\frac{N_{\mathrm{Na}}^* N_{\mathrm{Na}}}{\sqrt{N_{\mathrm{Cd}}^* N_{\mathrm{Cd}}}} = K_{\mathrm{Na-Cd}}\frac{p_{\mathrm{Na}}(c_{\mathrm{Na}}^* - c_{\Pi\mathrm{Na}}) + c_{\Pi\mathrm{Na}}}{\sqrt{p_{\mathrm{Cd}}(c_{\mathrm{Cd}}^* - c_{\Pi\mathrm{Cd}}) + c_{\Pi\mathrm{Cd}}}} \tag{10}$$

$$N_{\mathrm{Na}}^* N_{\mathrm{Na}} + N_{\mathrm{Pb}}^* N_{\mathrm{Pb}} + N_{\mathrm{Cd}}^* N_{\mathrm{Cd}} = N_0(z) \tag{11}$$

where

$$\left.\begin{aligned} & p_{ej} = \frac{Lu^*}{D_j} \\ & f = \frac{u}{u^*} \end{aligned}\right\} \tag{12}$$

the initial and boundary condition are converted as follows.

Initial condition

$$\left.\begin{aligned} \tau = 0\ ;\quad & P_j(\xi,\ 0) = \frac{c_{j0}(z) - c_{\Pi j}}{c_j^* - c_{\Pi j}} \\ & N_j(\xi,\ 0) = \frac{s_{j0}(z)}{N_j^*} \end{aligned}\right\} \tag{13}$$

boundary condition

$$\left.\begin{aligned} &\xi = 0; \quad P_j(0,\ \tau) = \frac{\varphi_j(t) - c_{\Pi j}}{c_j^* - c_{\Pi j}} \\ &\xi = 1; \quad \frac{\partial p_j(1,\ \tau)}{\partial \xi} = 0 \end{aligned}\right\} \tag{14}$$

Where $P_j,\ N_j$ are dimensionless concentrations of *j* ion in soil moisture and absorbing complex.

2. Deciding the diffusion coefficient

The mass flow q_z is zero at *z*=0. then

$$D_j(t)\frac{\partial c_j}{\partial z} = u(c_j(0,\ t) - c_{\Pi j}) \tag{15}$$

Let's convert Eq. (15) by Eq. (7) into dimensionless quantity, then

$$D_j(t)\frac{\partial p_j}{\partial \xi} = uLp_j(0,\ \tau) \tag{16}$$

Let's convert $\frac{\partial p_j}{\partial \xi}$ into a difference schema and arrange in order by $D_j(t)$, then

$$D_{ji}^{s+1} = \frac{2h}{uL}\frac{p_{j0}^{s+1}}{p_{j2}^{s+1} - 4p_{j1}^{s+1} + 3p_{j0}^{s+1}} \tag{17}$$

One can predict using Eq. (17) and Eq. (7)—(14).

At *s*+1-time step, an initial approximation of the D_{ji}^{s+1} are as follows.

$$[D_{ji}^{s+1}]^k = \frac{1}{2}\frac{p_{j0}^{s+1}}{Lu} \tag{18}$$

At three points in the research area, measured value, predicted value and error of the lead and cadmium are as follows. Table 1.

Table 1. Measured value, predicted value and error of the lead and cadmium at three points in the research area

point	Land category	Soil depth /cm	Heavy metals					
			Pb			Cd		
			measured value /(mg kg^{-1})	predicted value /(mg kg^{-1})	error/%	measured value /(mg kg^{-1})	predicted value /(mg kg^{-1})	error /%
1	Paddy field	30	247	263	6.48	12.9	11.73	9.07
		60	248	259	4.44	4.85	4.57	5.77
2	Corn field	30	255	271	6.27	4.75	4.29	9.68
		60	248	211	14.92	4.48	4.15	7.37
	Vegetable field	30	281	238	15.30	4.45	4.79	7.64
	Paddy field	30	382	352	7.85	5.58	5.92	6.09
3	Paddy field	30	219	269	22.83	4.96	4.13	16.73
		60	238	227	4.62	2.82	2.31	18.09
	Corn field	30	235	245	4.26	3.16	3.71	17.41
		60	215	254	18.14	3.46	3.12	9.83
	Vegetable field	30	227	247	8.81	4.32	4.58	6.02

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After word

The error of the measured value and predicted value of lead and cadmium are 10.36% and 10.34%. Therefore, this method can be used for the diffusion prediction of the heavy metals in soil.

References

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