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博士論文

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溶質在土壤中流散之推估
Prediction on Solute Dispersion in Soils

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摘要

混合取代用途甚廣，對於溶質流散、鹽分移動，採用流散方程式可預估的非常準確。問題是應用本項技術有三個先決條件要先滿足：第一是在試驗前，土壤中必須不含使用之追蹤物，故需事前淋洗，頗費時日。其次是預估流散係數必須另做一條無反應之突破曲線，故得再做一次輔助試驗。最後是預估有反應之突破曲線需加入交換方程式，而交換方程式之確立，尚需實驗求得。

本研究即嘗試利用數學推導及應用熱力學原理，處理以上三項先決條件，得以免除繁複之輔助試驗及測定。試驗結果顯示，三種土壤含原追蹤物之濃度不高，不淋洗亦可直接由突破曲線計算得流散係數，其公式爲

$$D=\left(1-\frac{B}{R}\right)^2 \frac{L}{\pi} \bar{v}$$

流散係數求得後，交換方程式中之K可應用熱力學原理計算，其公式：

$$\Delta\bar{G}^0=\Delta\bar{H}^0-T\Delta\bar{S}^0$$

及

$$\Delta\bar{G}^0=-RT\ln K$$

至於另一參數c，可以電化學理論推測：

$$c=\exp\left(-\frac{zF\psi+\Phi}{RT}\right)$$

配合電腦程式模擬，即可充分描述溶質在土壤中之流散現象。

Summary

The miscible displacement technique has been applied in many fields of study. Solute dispersion through a porous medium can be accurately predicted by the dispersion equation. However, there are three requirements must be met while using this technique: (1) the porous medium should contain no tracer element, (2) it requires a nonreactive breakthrough curve for determining the dispersivity, D, and (3) it is necessary to establish an exchange function if there are interactions between the porous medium and the tracer. The miscible displacement technique is, therefore, a time consumed process. The application through mathematical and thermodynamic treatments is used in this research in order to simplify the process..

The result shows that three soils though contain a few tracer element can still predict the dispersivity, D, very well as follows

$$D = \left(1 - \frac{B}{R}\right)^2 \frac{L}{\pi} \bar{v}$$

Finally, thermodynamics and electrochemistry are used to find the parameters K, c in the exchange function by the following equatios:

$$\Delta\bar{G}^0 = \Delta\bar{H}^0 - T\Delta\bar{S}^0 \; ; \; \Delta\bar{G}^0 = -RT \ln K$$

and

$$c = \exp\left(-\frac{zF\psi + \Phi}{RT}\right)$$

which is needed to predict the solute dispersion phenomena in soils.