裂隙中双分子反应性溶质运移实验与模拟

刘雅静，刘咏，马雷，钱家忠

(合肥工业大学地下水科学与工程研究所，合肥，230009，Email: qianjiazhong@hfut.edu.cn)

摘要：地下水环境中的化学作用对溶质运移具有重要的影响，然而对于双分子反应性溶质运移的研究,以往大多是在多孔介质中展开的,并且传统的对流弥散方程不能很好的解决“过度预报”生成物浓度以及生成物“拖尾”问题。为了揭示双分子反应性溶质在裂隙介质中的运移机理，论文以苯胺（AN）和 1,2-萘醌-4-磺酸钠（NQS）为例，开展了单个裂隙中双分子反应性溶质运移实验与模拟研究，重点研究了裂隙开启度、水流属性以及运移路径的影响，建立了考虑随时间衰减的反应性溶质运移数学模型(ADRE)并进行数值求解，进行了模型参数分析，与现有的对流弥散方程(ADE)模型及随机的截断幂函数模型(TPL)进行比较，得到 ADRE 模型对溶质运移峰值浓度预报精度较高，而不能很好捕捉“拖尾”现象，TPL 模型捕捉“拖尾”现象的能力高于 ADRE 模型,其机理有待进一步研究[Grants: 41831289; 41877191]。

关键词：双分子反应；溶质运移；裂隙；拖尾；过度预报

Experimental and simulation of bimolecular reactive solution transport in fractures

LIU Ya-jing, LIU Yong, MA Lei, QIAN Jia-zhong

(Institute of groundwater science and engineering, Hefei University of Technology, Hefei, 230009.
Email: Liuyong@hfut.edu.cn; qianjiazhong@hfut.edu.cn)

Abstract: Chemical action in groundwater environment has an important impact on solute transport. However, most of the studies on bimolecular reactive solute transport have been carried out in porous media in the past, and the traditional advection-dispersion equation (ADE) can not solve the problem of "over-prediction" of the concentration of products and "long-tail" of products. In order to reveal the transport mechanism of bimolecular reactive solutes in fracture

media, In this paper, we take the bimolecular reactive as an example，the aniline (AN) and 1,2-napthoquinone-4-sulfonic (NQS) acid were used as the chemical reactants. The effects of fracture aperture, flow properties and transport path were mainly studied. A mathematical model of reactive solute transport (ADRE) considering time decay was established and solved numerically. The parameters of the model were analyzed. Compared with advection-dispersion equation (ADE) model and the stochastic Truncated Power-law (TPL) function model, it is concluded that the ADRE model is more precise in predicting the peak concentration of solute transport, but the "long-tail" can not be fitted well. The TPL model is better than ADRE model to fit the "long-tail", and its mechanism needs to be studied further [Grants: 41831289；41877191].

Key words：Bimolecular reactive; Solute transport; Fracture; “Long tail”; Over-prediction.