Simulation of Radionuclide Transport in Fractured Porous Media

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Abstract

High-level radioactive waste (HLW) contains hazardous materials that can remain radioactive for thousands of years. Deep geological disposal with a multi-barrier system is a widely accepted international approach for final disposal. These repositories are engineered to maintain stability and security over geological timescales. Safety assessments and transport simulations are essential to ensure effective containment and isolation of these radioactive materials, minimizing radiation exposure risks to humans and the environment. Especially when the host rock is hard rock (e.g., granite), simulations of radionuclide transport considering chemical reactions in fractured porous media are crucial for safety evaluation.

This study aims to develop a model for simulating radionuclide transport in fractured porous media. PHREEQC is anticipated for use in the chemical reaction module, with preliminary testing underway. Parameters for chemical simulations are primarily obtained from literature and experiments. Through literature review, this study not only collected thermodynamic parameters related to nuclear species but also used PHREEQC to reproduce experimental results. Results show that PHREEQC can effectively replicate experimental results under known conditions, making it a valuable and practical geochemical simulation program. The developing model aims to enhance the accuracy and reduce uncertainty in radionuclide transport simulations in fractured porous media. It also seeks to enhance confidence in safety evaluations for deep geological disposal, ensuring the long-term safety and effectiveness of HLW final disposal.

Keywords: Radionuclide transport, Fractured porous media, Chemical reaction simulation, PHREEQC.

裂隙-孔隙介質內的放射性核種傳輸模擬

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摘要

高放射性廢棄物含有許多具有高放射性與高毒性之物質。為確保高放射性廢棄物最終處置的安全性，國際上多採用深層地質處置與多重障壁系統的設計，並搭配安全評估和核種傳輸模擬，以確保其能有效隔離和圍阻這些放射性物質，最大限度地減少人類和環境的輻射暴露風險。尤其當處置母岩為堅硬岩體(如：花崗岩)時，溶質傳輸主要透過裂隙傳導，因此更需考慮裂隙-孔隙介質中放射性核種化學反應傳輸模擬。

本研究目的在開發一種用於模擬裂隙-孔隙介質中放射性核種傳輸的程式。該程式預計使用 PHREEQC 作為化學反應組件，目前正在進行初步測試。化學模擬所需的參數主要透過文獻蒐集和實驗獲得。透過文獻資料，本研究不僅收集了與核種相關的熱力學參數，也利用 PHREEQC 重現實驗結果。結果顯示，PHREEQC 可以有效再現已知條件下的實驗結果，使其成為有實用的地球化學模擬程式。本研究希望所開發的程式可以提高裂隙-孔隙介質中放射性核種傳輸模擬的準確性，並減少不確定性，以增強深層地質處置安全評估的信心，確保高放射性廢棄物最終處置的長期安全性和有效性。

關鍵字： 放射性核種傳輸、裂隙-孔隙介質、化學反應模擬、PHREEQC