



Modeling of Ion Chromatography in a Novel Microfluidic Device

Experiments and simulations at the microscale can be used to accelerate the optimization of rare earth element separation via ion exchange. Fluorescence data collected directly on ion exchange resin is used in this work to validate a model for ion exchange of rare earths in a microfluidic device.

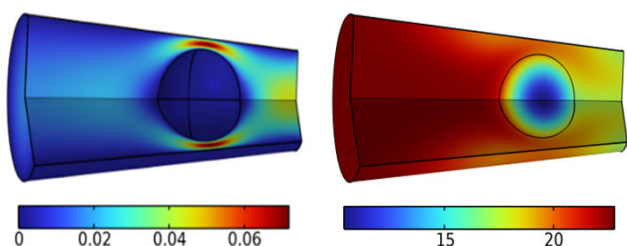
Samuel Hartness¹, Zachary Magnuson¹, Rebecca Carter-Torcivia¹, Katherine Koh¹, Christopher Sobecki¹

1. Savannah River National Laboratory, Aiken, SC, USA.

Introduction

Efficient separation and recovery of rare earth elements (REE) from waste streams is essential to ensure sustainable supply and developing alternative sources to meet increasing demands. Ion exchange (IX) chromatography remains a widely used and highly effective method for REE separation. Recent advances in 3D printing microfluidic devices (MFD) enable novel platform fabrication for rapid online monitoring in microgram scale and separating REE using IX resins. Innovative MFD experiments and simulations offer an increased throughput to accelerate optimization of REE separation.

The current work investigated neodymium separation from a strong acid cationic resin, Dowex 50W-X8, in a new microfluidic system [1]. Nd was used for evaluation of the MFD and initial simulations considering the molecule can not only adsorb light in the UV-Vis region but also fluoresces, allowing for unique on-line analysis of the IX process in the microfluidic device in the work of Magnuson et al. [1]. The fluorescence data captured directly on the resin bead allowed for a time profile of adsorption on the bead to be captured, which was used in the current study for validation. The unique dataset and microfluidic approach also allowed for a direct analysis and evaluation of the resin bead via simulations.



Methodology

Transport of Diluted Species in Porous Media and Laminar Flow Physics were used to simulate the mass transport around and inside of the resin bead. Fickian diffusion was used to simulate transport into and inside the bead with the addition of a thin film diffusion layer on the resin surface. To capture the competition between cations in solution and the capacity of the resin, a competitive Langmuir isotherm was used [2]. Simulations are broken into loading and elution stages due to the different flowrates and chemical concentrations.

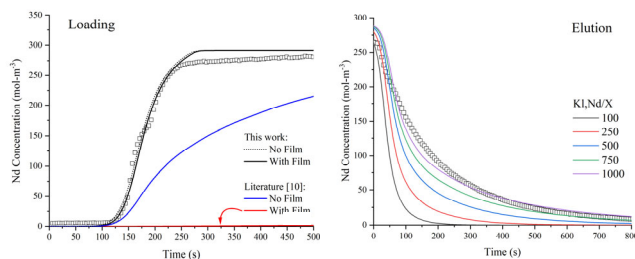
$$\nabla \cdot \mathbf{J}_i + \mathbf{u} \cdot \nabla c_i = R_i + S_i, \quad \mathbf{J}_i = -(D_{D,i} + D_{e,i}) \nabla c_i,$$

$$Q_{e,i} = Q_{m,i} \frac{K_{L,i} C_{e,i}}{1 + \sum_{j=1}^N K_{L,j} C_{e,j}}$$

Velocity ($\text{m}\cdot\text{s}^{-1}$) profile on the left and Nd concentration ($\text{mol}\cdot\text{m}^{-3}$) profile on the right taken during loading simulations with a flowrate of $100 \mu\text{L}\cdot\text{min}^{-1}$.

Results

The competitive Langmuir adsorption model was validated against experimental data. The adaptive model successfully predicted Nd loading profiles up to 90% bead capacity range. The use of higher diffusion rates than anticipated was required to match experiments on a single Dowex 50W-X8 bead. This critical finding suggests that evaluation of resins for REE separation using continuous flow and a single resin bead in a microfluidic device can be done significantly faster than evaluation with full columns or batch applications, providing a great screening tool to accelerate REE separations using IX. The modeling approach required fewer input parameters and less experimental calibration, which streamlines future simulation efforts.



Nd loading (left) and elution (right) profiles. Loading profiles compare diffusion parameters in this work to literature values for intraparticle and film diffusion, illustrating improved model agreement with experimental data when using higher diffusion rates. Nd elution profiles are shown using different H^+ affinity values, illustrating improved model agreement with experimental data when using a lower H^+ affinity. An affinity ratio of 1000:1 for Nd and H^+ resulted in the closest approximation. Squares are experimental data from Magnuson et al. [1].

REFERENCES

- [1] Magnuson, Z., et al., Direct Monitoring of a Single Ion Exchange Resin Bead in a Microfluidic Device [In Preparation]. 2026, Savannah River National Lab.
- [2] Yang, R.T., Gas Separation by Adsorption Processes. 1997: Imperial College Press.



Savannah River National Laboratory®