§9. Lithium Isotope Separation with Displacement Chromatography Using Cryptand Polymer

Sugiyama, T., Sugiura, K. (Nagoya Univ.), Tanaka, M.

i) Introduction

Although natural lithium contains only about 7.6 % of $^6\text{Li}$, isotopic enrichment of $^6\text{Li}$ up to 30-90 % is required for adequate tritium breeding in many fusion reactor concepts. Displacement chromatography using a cryptand resin is one of the suitable methods for a large-scale production of the enriched $^6\text{Li}$, because a scale-up of a process seems easy and energy consumption is relatively small. In the previous study we evaluated the separative performance of the cryptand resin by experiments and numerical simulation. The purpose of the present study is to investigate the relationship between HETP value and the radius of the resin particle in order to improve the separative performance of Li isotope separation.

ii) Numerical analysis

Fundamental equations, which describe transport phenomena in the chromatographic column are

$$\frac{\partial C_i}{\partial t} = E \frac{\partial^2 C_i}{\partial z^2} - u \frac{\partial C_i}{\partial z} - \frac{k_s a_v}{\varepsilon_v} (q^*_i - q_i) \quad \text{and} \quad \frac{\partial q_i}{\partial t} = k_s a_v(q^*_i - q_i).$$

$C_i$: Concentration in the liquid phase [mol cm$^{-3}$]
$E$: Dispersion coefficient [cm$^2$ s$^{-1}$]
$k_s a_v$: Mass transfer coefficient [s$^{-1}$]
$q_i$: Concentration in the resin phase [mol cm$^{-3}$]
$t$: Time [s]
$u$: Velocity [cm s$^{-1}$]
$z$: Axial position [cm]
$\varepsilon_v$: Porosity [-]
$q^*_i$: Equilibrium state

Diffusion in the resin particle was assumed to be a rate-determining step and the mass transfer coefficient was evaluated as $k_s a_v = 15D/r_o^2$, where $r_o$ is the radius of the resin particle. Finite differential forms of these equations were solved numerically and concentration profiles in the column were obtained. Values of HETP were determined numerically using the concentration profiles obtained. The parameters used in the calculation were summarized in Table I.

iii) Results and discussion

Figure 1 shows the concentration and the isotopic ratio of lithium isotopes around the frontal edge of the chromatogram. The shape of the frontal edge became steeper with decreasing in the radius. This result implies that the diffusive resistance becomes small with the radius. The values of HETP were plotted against the particle diameter in Fig. 2. The numerical calculation clearly shows that the HETP value becomes small with the radius of the resin particle.

iv) Conclusion

In order to improve the separative performance of Li isotope separation with displacement chromatography, the relationship between HETP value and the radius of the resin particle was numerically investigated. It was found that the HETP value becomes small with the radius of the resin particle. In the case of 100 μm in the radius the HETP value became one-sixth of that for 350 μm, which is a typical value of particle radius commercially obtained.

Table I: Parameters for numerical calculation

<table>
<thead>
<tr>
<th>No. in Fig. 1</th>
<th>Polymer diameter [mm]</th>
<th>Dispersion factor [cm$^2$ s$^{-1}$]</th>
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</thead>
<tbody>
<tr>
<td>1a</td>
<td>0.10</td>
<td>5.5×10$^{-4}$</td>
</tr>
<tr>
<td>2a</td>
<td>0.15</td>
<td>8.3×10$^{-4}$</td>
</tr>
<tr>
<td>3a</td>
<td>0.20</td>
<td>1.1×10$^{-3}$</td>
</tr>
<tr>
<td>4a</td>
<td>0.25</td>
<td>1.4×10$^{-3}$</td>
</tr>
<tr>
<td>5a</td>
<td>0.30</td>
<td>1.7×10$^{-3}$</td>
</tr>
<tr>
<td>6</td>
<td>0.35</td>
<td>1.9×10$^{-3}$</td>
</tr>
</tbody>
</table>

Fig. 1: Effect of the particle diameter on the profiles of Li isotope ratio and Li concentration

Fig. 2: Relationship between HETP and particle diameter