Dispersion in LFR

2dayclean

2025/10/08

1. Tabular reactor에서의 dispersion을 고려한 mass conservation equation은 다음과 같이 나타난다.

$$\frac{\mathrm{D}C}{\mathrm{D}t} = \mathcal{D}_{AB}\nabla^2 C$$

로부터,

$$\frac{\partial C}{\partial t} + u(r)\frac{\partial C}{\partial z} = \mathcal{D}_{AB}\left\{\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C}{\partial r}\right) + \frac{\partial^2 C}{\partial z^2}\right\}$$

가 된다.

2. 이제, $z^* = z - Ut$와 같이 변환하자. (U는 Hagen-Poiseuille flow의 average velocity, $U_{\max}$의 절반.) 그러면, 다음과 같이 식을 쓸 수 있다.

$$\left(\frac{\partial C}{\partial t}\right)_{z^*} + [u(r) - U]\frac{\partial C}{\partial z^*} = \mathcal{D}_{AB}\left\{\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C}{\partial r}\right) + \frac{\partial^2 C}{\partial z^{*2}}\right\}$$

3. Radial한 방향으로의 평균을 낸 $\bar{C}$를 다음과 같이 정의하자.

$$\bar{C}(z,t) = \frac{1}{\pi R^2}\int_0^R C(r,z,t)2\pi r dr$$

4. 이제, (2)의 식을 근사하기 위하여, 다음과 같은 조건을 생각하자.

   (a) $[u(r) - U]\dfrac{\partial C}{\partial z^*} \gg \mathcal{D}_{AB}\dfrac{\partial^2 C}{\partial z^{*2}}$

   (b) $\left(\dfrac{\partial C}{\partial t}\right)_{z^*} \approx 0$

   (c) $\dfrac{\partial C}{\partial z^*} \approx \dfrac{\partial \bar{C}}{\partial z^*}$

5. 따라서, (2)의 식은 (4)의 근사로부터 다음과 같은 전개를 얻는다.

$$[u(r) - U]\frac{\partial \bar{C}}{\partial z^*} = \mathcal{D}_{AB}\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C}{\partial r}\right)$$
$$\therefore r\frac{\partial C}{\partial r} = \frac{1}{\mathcal{D}_{AB}}\frac{\partial \bar{C}}{\partial z^*}\int_0^r U\left[r - 2\frac{r^3}{R^2}\right]dr + K_1$$

$r = 0$에서 $\dfrac{\partial C}{\partial r}$은 finite하므로 $K_1 = 0$이다.

$$\begin{aligned}
r\frac{\partial C}{\partial r} &= \frac{U}{\mathcal{D}_{AB}}\frac{\partial \bar{C}}{\partial z^*}\left[\frac{1}{2}r^2 - \frac{1}{2}\frac{r^4}{R^2}\right] \\
\frac{\partial C}{\partial r} &= \frac{U}{\mathcal{D}_{AB}}\frac{\partial \bar{C}}{\partial z^*}\left[\frac{1}{2}r - \frac{1}{2}\frac{r^3}{R^2}\right] \\
C(r,z,t) &= \frac{U}{\mathcal{D}_{AB}}\frac{\partial \bar{C}}{\partial z^*}\int_0^r \frac{1}{2}r - \frac{1}{2}\frac{r^3}{R^2}dr \\
&= \frac{R^2 U}{4\mathcal{D}_{AB}}\frac{\partial \bar{C}}{\partial z^*}\left[\left(\frac{r}{R}\right)^2 - \left(\frac{r}{R}\right)^4\right] + K_2
\end{aligned}$$

6. 이제 $\bar{C}$의 정의로부터 다음을 얻는다.

$$
\begin{aligned}
\bar{C}(z,t) &= \frac{1}{\pi R^2}\int_0^R C(r,z,t)2\pi r dr \\
&= \frac{2}{R^2}\frac{R^2 U}{4\mathcal{D}_{AB}}\frac{\partial \bar{C}}{\partial z^*}\int_0^R \left[\left(\frac{r}{R}\right)^2 - \left(\frac{r}{R}\right)^4\right] r dr + K_2 \\
&= \frac{R^2 U}{12\mathcal{D}_{AB}}\frac{\partial \bar{C}}{\partial z^*} + K_2 \\
K_2 &= \bar{C} - \frac{R^2 U}{12\mathcal{D}_{AB}}\frac{\partial \bar{C}}{\partial z^*} \\
\therefore C(r,z,t) &= \bar{C} + \frac{R^2 U}{4\mathcal{D}_{AB}}\frac{\partial \bar{C}}{\partial z^*}\left[-\frac{1}{3} + \left(\frac{r}{R}\right)^2 - \frac{1}{2}\left(\frac{r}{R}\right)^4\right]
\end{aligned}
$$

7. 이제, (2)의 식으로부터, 양변을 averaging하여 다음을 얻는다.

$$
\begin{aligned}
&\left(\frac{\partial \bar{C}}{\partial t}\right)_{z^*} + \frac{1}{\pi R^2}\int_0^R U\left[1 - 2\left(\frac{r}{R}\right)^2\right]\left[\frac{\partial \bar{C}}{\partial z^*} + \frac{R^2 U}{4\mathcal{D}_{AB}}\frac{\partial^2 \bar{C}}{\partial z^{*2}}\left\{-\frac{1}{3} + \left(\frac{r}{R}\right)^2 - \frac{1}{2}\left(\frac{r}{R}\right)^4\right\}\right] 2\pi r dr \\
&= \mathcal{D}_{AB}\frac{1}{\pi R^2}\int_0^R 2\pi \frac{\partial}{\partial r}\left(r\frac{\partial C}{\partial r}\right) dr + \mathcal{D}_{AB}\frac{\partial^2 \bar{C}}{\partial z^{*2}}
\end{aligned}
$$

8. Boundary condition으로, $r = 0$에서 $r\dfrac{\partial C}{\partial r} = 0$이고 $r = R$에서 $r\dfrac{\partial C}{\partial r} = 0$(no flux)이므로, (7)의 식은 다음과 같다.

$$
\left(\frac{\partial \bar{C}}{\partial t}\right)_{z^*} - \frac{1}{48}\frac{U^2 R^2}{\mathcal{D}_{AB}}\frac{\partial^2 \bar{C}}{\partial z^{*2}} = \mathcal{D}_{AB}\frac{\partial^2 \bar{C}}{\partial z^{*2}}
$$

9. 이제 $z^* = z - Ut$를 돌려보내면, 다음을 얻는다.

$$
\begin{aligned}
\frac{\partial \bar{C}}{\partial t} + U\frac{\partial \bar{C}}{\partial z} &= \mathcal{D}^*\frac{\partial^2 \bar{C}}{\partial z^2} \\
\mathcal{D}^* &:= \mathcal{D}_{AB} + \frac{U^2 R^2}{48\mathcal{D}_{AB}}
\end{aligned}
$$

이를 **Aris-Taylor Dispersion coefficient**라고 한다.