Colored dyes are used to impart color to an array of materials, and can be in the forms of pigments, dyes or ionized solutions. Dyes, which are organic, soluble, colored compounds, can be natural or synthetic, and are used in the textile, cosmetic, food, and pharmaceutical industries. The manufacturing of dyes has evolved from extractions of natural products, to an industrialized production of synthetic dyes, up to 7 x 10^6 tons/year. Dyes, or their degradation products in water can cause various human health disorders and can cause severe damage to various organs. Also, the presence of even trace amounts of dye in effluent is highly undesirable due to its esthetic pollution and perturbations in aquatic life. While there is a considerable amount of research for textile dye effluent wastewater treatment, toxic dyes produced by the cosmetic and personal care sector, remain yet to be investigated as diligently. It is widely hypothesized that adsorption can be efficiently employed for the removal of various toxic dyes from wastewater.

### Mathematical Model (Pore-level)

We begin our mathematical analysis of this CSTR with the microscopically species continuity equation for which the figure above illustrates the governing domain. The assumption that this is a long cylinder with one end sealed, omits the problem of convection in this particular region of the hydrogel bead. The following equation is the species continuity equation for the pore-level:

\[
\frac{\partial C_a}{\partial t} + D \left( \frac{\partial C_a}{\partial r} \right) + \frac{\partial^2 C_a}{\partial z^2} = 0
\]

Where:
- \( C_a \) is the concentration of dye
- \( D \) is the diffusion constant
- \( r, z \) is radial & axial directions, and time

**Boundary Conditions**

- No convection
- Steady state
- Angular symmetry
- Long-channel approximation

\[
C_{af} = C_{af}(r, z = 0)
\]

\[
\frac{\partial C_a}{\partial z} = 0
\]

\[
\frac{\partial C_a}{\partial r} = 0
\]

\[
D \frac{\partial^2 C_a}{\partial r^2} = K_{ca} \frac{1}{L}(C_a - C_{af})
\]

\[
C_{af} \text{ is the concentration of dye in the wastewater}
\]

\[
L \text{ is the length of the pore}
\]

\[
K_r \text{ is the reaction constant}
\]

\[
K_{na} \text{ is the adsorption constant}
\]

### Area-averaged Pore-level Equation

We apply the definition of area-averaged concentration to our initial SCE and evaluate this at the boundary conditions presented above. This mathematical analysis leads us to the following area-averaged equation for the pore-level:

\[
\frac{2}{R} \left( \frac{K_{ca}}{1 + K_{ad}C_a} \right) + D \frac{d^2 C_a}{dz^2} = 0
\]

We can then derive the pellet-level equation by upscaling the area-averaged pore-level equation. The pellet-level equation is as follows:

\[
\epsilon \left( \frac{KC_a}{1 + K_{ad} C_a} \right) + \epsilon D_{eff} \frac{d^2 C_a}{dz^2} = 0
\]

Where:
- \( \epsilon \) is the porosity of the hydrogel bead
- \( D_{eff} \) is the effective diffusivity factor

### Fluid-level Equation

The species mass conservation equation for the fluid phase is as follows:

\[
\frac{NC_i}{dt} = \nabla N \cdot \nabla + R_i' (C_i, T)
\]

Where:
- \( N \) is the molar flux of A in the fluid
- \( R_i' \) is the reaction function of A in the fluid

### References