Modeling the Removal of Cosmetic Dyes Using Hydrogel Materials in a CSTR

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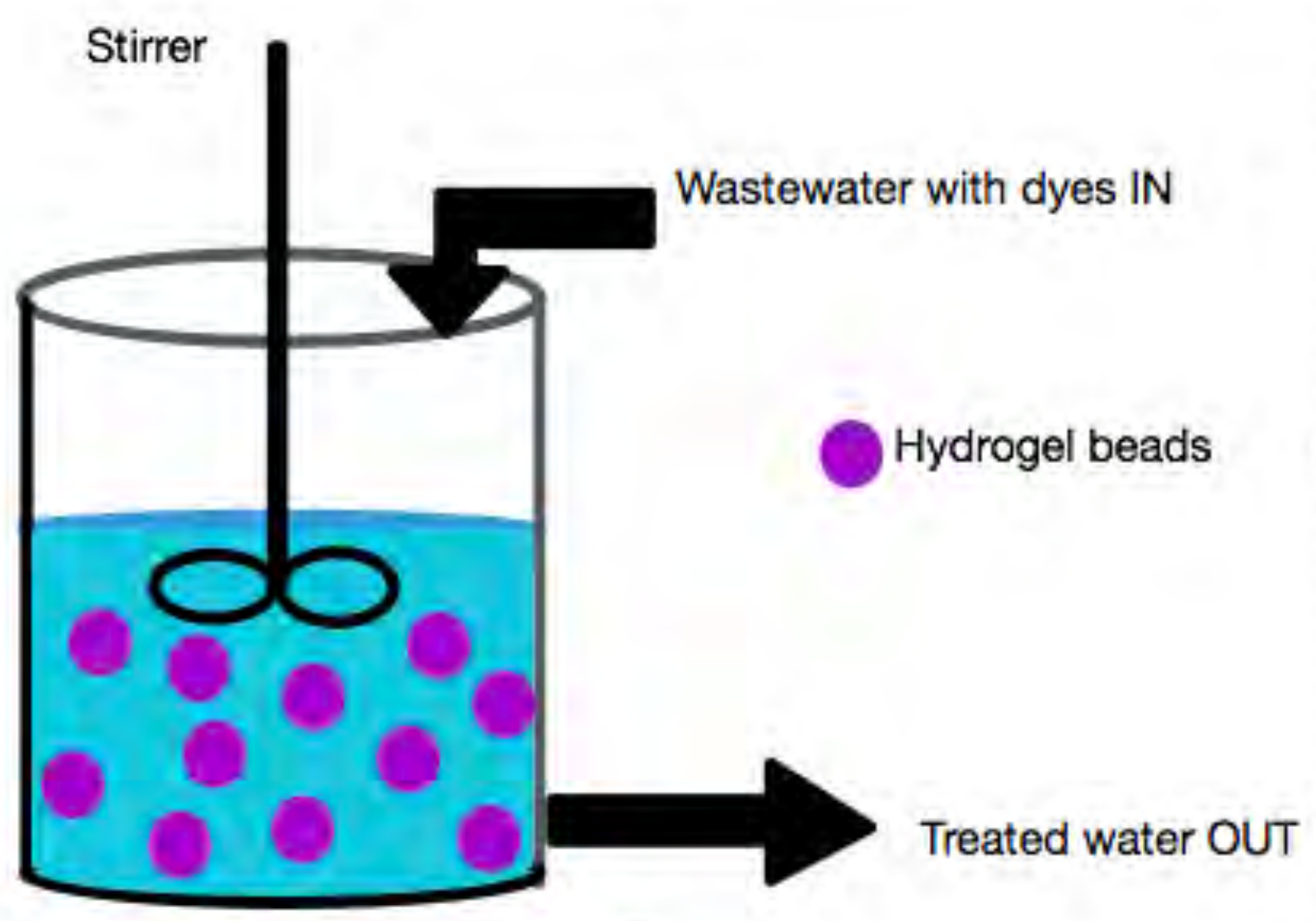
Motivation and Need for Research



Colorants 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 10^5 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.

Research Strategy

- STEP 1 — Reactor Schematic
- STEP 2 — Literature Investigation
- STEP 3 — Mathematical Model (pore-level)
- STEP 4 — Area-averaging
- STEP 5 — Fluid Level (SCE)

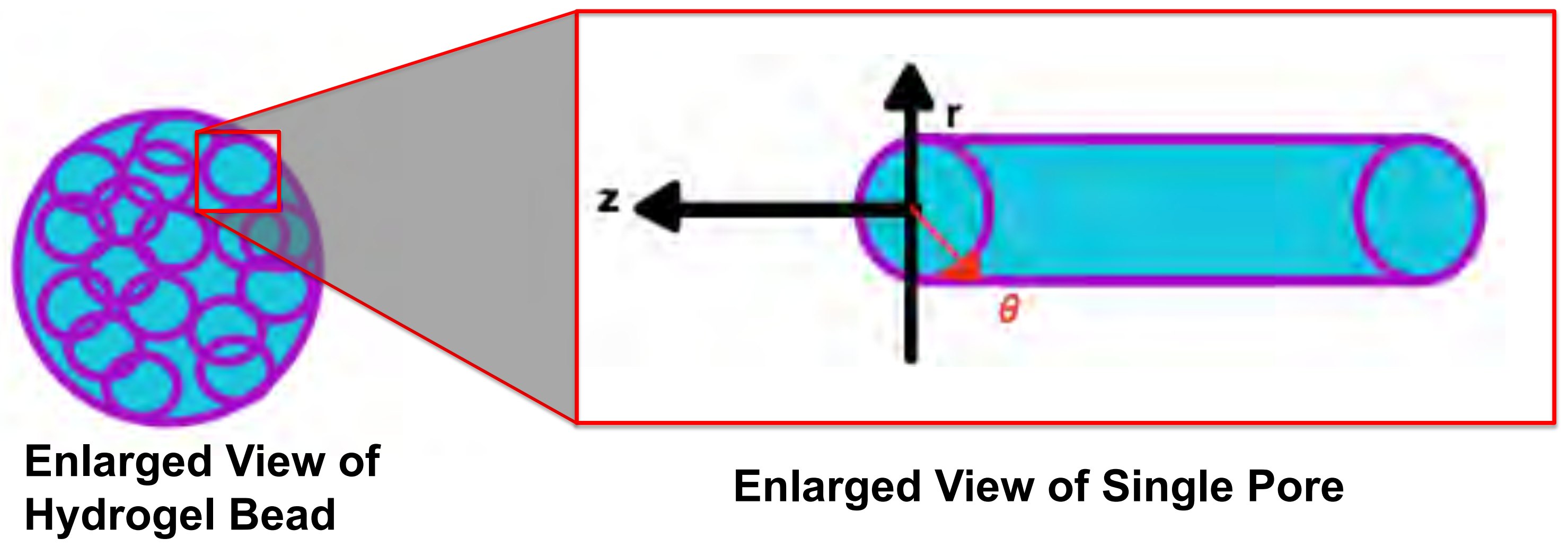
This research follows the pedagogical sequential steps based on Arce, et. al. The Catalytic Pellet[7], which has been modified by including steps relevant to this research (refer to the figure below). The reactor schematic is depicted in figure above.

Literature Investigation

Ref. #	Type of dyes	Health risks
1	Permanent hair dyes	Carcinogenicity
2	Hair dyes, reactive dyes, textile dyes	Contact urticaria
3	Quinoline Yellow	DNA damage
4	Hair dyes	Skin irritation and allergy, cancer

Ref. #	Material adsorbed	Type of hydrogel
5	Crystal violet	Hydrogel beads
6	Cationic dyes and heavy metals	P(DMAM co-Ana)

Results



Enlarged View of Hydrogel Bead

Enlarged View of Single Pore

Mathematical Model (Pore-level)

We begin our mathematical analysis of this CSTR with the microscopic 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:

$$\frac{\partial C_A}{\partial t} = D\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_A}{\partial z}\right) + \frac{\partial^2 C_A}{\partial z^2}\right]$$

C_A is the concentration of dye
D is the diffusion constant
r, z, t is radial & axial directions, and time

Assumptions

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

Boundary Conditions

$$C_A = C_{Af} \ at\ z = 0$$

$$\frac{\partial C_A}{\partial z} = 0 \ at\ z = L$$

$$\frac{\partial C_A}{\partial r} = 0 \ at\ r = 0$$

$$D\frac{\partial C_A}{\partial r} = \frac{KC_A}{1+K_{ads}C_A} \ at\ r = R$$

C_{Af} is the concentration of dye in the wastewater
L is the length of the pore
K is the reaction constant
K_{ads} 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:

$$\frac{2}{R}\left(\frac{KC_A}{1+K_{ads}C_A}\right) + D\frac{d^2\langle C_A\rangle}{dz^2} = 0$$

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

$$\varepsilon\frac{2}{R}\left(\frac{KC_A}{1+K_{ads}C_A}\right) + \varepsilon D_{eff}\frac{d^2\langle C_A\rangle}{dz^2} = 0$$

ε 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:

$$\frac{\partial C_A^f}{\partial t} = \vec{\nabla}.\overrightarrow{N_A^f} + R_A^f(C_A^f, T)$$

N_A^f is the molar flux of A in the fluid
R_A^f is the reaction function of A in the fluid

Discussion

The area-averaging approach used to obtain the pore-level equation was based on the closure approach, Arce, et. al. The Catalytic Pellet[7], where a pedagogical strategy was constructed to obtain the macroscopic equations. Thus, we have obtained the pore-level equation, which is then area-averaged to obtain a new equation which can then be up-scaled using the limiting case $K_{add}C_A^s \ll 1$ to derive the pellet-level equation. This equation describes the area-average concentration of dye within each hydrogel bead in the CSTR. Finally, a macroscopic equation for the fluid phase in the CSTR has also been listed, and was based on Allred, A. Nastasia, et al. Cilindro Rotador[8].

Pore-level Equation

$$\frac{\partial C_A}{\partial t} = D\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_A}{\partial z}\right) + \frac{\partial^2 C_A}{\partial z^2}\right]$$

Area-averaged Pore-level Equation

$$\frac{2}{R}\left(\frac{KC_A}{1+K_{ads}C_A}\right) + D\frac{d^2\langle C_A\rangle}{dz^2} = 0 \xRightarrow{K_{add}C_A^s \ll 1} \frac{2K}{R}\langle C_A\rangle + D\frac{d^2\langle C_A\rangle}{dz^2} = 0$$

Pellet-level Equation

$$\varepsilon\frac{2K}{R}\langle C_A\rangle + \varepsilon D_{eff}\frac{d^2\langle C_A\rangle}{dz^2} = 0$$

Species Mass Conservation Equation (SCE) for Fluid-level

$$\underbrace{\cancel{\frac{\partial C_A^f}{\partial t}}}_{\text{Steady State}} = \vec{\nabla}.\overrightarrow{N_A^f} + \underbrace{\cancel{R_A^f(C_A^f, T)}}_{\text{No Bulk Reaction}} \Rightarrow \vec{\nabla}.\overrightarrow{N_A^f} = 0$$

After Up-Scaling In The Fluid Domain

$$Q\left[\langle C_A^f\rangle - \langle C_A^0\rangle\right] = Kg\left[\langle C_A\rangle|_{z=0} - \langle C_A^f\rangle\right]$$

Conclusions And Future Work

In light of the results obtained from the pore-level, pellet-level, and fluid-level domains we can then conclude that a macroscopic equation, relevant to this research, must be derived for the fluid phase in order to calculate the dye adsorption capacity of the hydrogel beads. This will then enable us to validate this technology for implementation commercially. We hope that the future results of this research can make this technology a viable option for dye removal from wastewater. This dye removal technique can also be applied to other contaminants that obey the Langmuir Adsorption Isotherm, such as heavy metals and reactive dyes.

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