Modeling Chemical Reactors from First Principles: The Batch Photocatalytic Reactor

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Motivation and Relevance of Research

In the modeling of isothermal chemical reactors, the specialization of the species continuity equation (for a given reactor domain) is one of the key aspects the modeler needs to address. A helpful starting point is the identification of proper simplifying assumptions for the various phenomena involved in the reaction process; these may be related to the type of reactor used, the type of reactant mixture present in the system, and the chemical reactions taking place, among other aspects. In the case of a photocatalytic reactor, the modeling of the radiation field must be coupled with the species continuity equation. The reason behind this need is based upon the dependence of the reaction rate on the radiation field intensity. This field can be modelled on the basis of the photon balance equation. In this contribution, we will outline a systematic approach to derive the up-scaled equations for a batch photocatalytic reactor with degradation taking place at the photocatalytic thin film surface located at the wall of the reactor. Both the species continuity equation and the photon conservation equation will be upscaled using a volumetric averaging approach in order to derive the engineering reactor equations. Furthermore, the model solution will be illustrated with conversion results of a biomedical contaminant, i.e., acetaminophen, and comparison with experimental results. Suggestions for future work will be also highlighted.

Methodology

Description of system:

You can see a visual description of the system above. This system is a cylindrical system that uses a radiation field to purify water that is contaminated by Acetaminophen.

Characterizing the system:

We have a isothermal, isobaric batch reactor that is at steady state and has a constant volume. We can also assume that the solution is well mixed, and radiation transport only occurs in the direction towards the photocatalytic film. We can neglect the reflection of photons and the scattering of protons. Our last assumptions are that reactions only occur at the wall of the reactor at the interface.

Equations we are using:

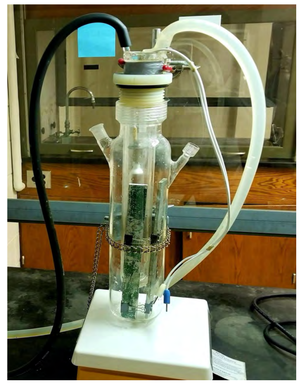
Our equations are as follows: Microscopic Species Mass Equation, Macroscopic Species Mass Equation, Macroscopic Radiation Conservation Equation, and Microscopic Radiation Equation, all shown on the right.

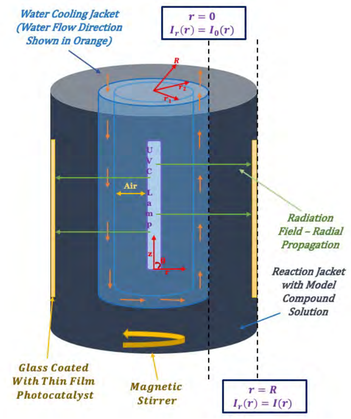
Solving for our values:

We will be solving values for three different scenarios: 6 layers of TiO, 8 layers of TiO, and 10 layers of TiO (TiO is our photocatalyst in this experiment). Once the material-dependent linear attenuation coefficient and the apparent reaction rates are determined experimentally, all needed variables will be known and the model can be tested to find values for the final species concentration.

Model of our system

Equations representing the species mass conservation and radiation were derived using the schematic (below) of the TTU reactor.





Conservation of Species Mass

Assumptions	Microscopic Species Mass Conservation	Resulting Macroscopic Species Mass Equation
- Batch Reactor - Transient - Constant Physical Properties - Constant Volume - Isothermal - Isobaric - Well-Mixed - Wall Reactions Only	$\frac{\partial C_A}{\partial t} = \vec{V} \cdot \vec{N_A} + R_A(C_A, T)$ - $\mathbf{C_A}$: concentration of species A - **t**: time - $\mathbf{N_A}$: total molar flux - $\mathbf{R_A}$: reaction rate in fluid - **T**: temperature **Interface Boundary Condition** $\vec{N_A} \cdot \vec{N} = R_A(C_A, \phi(R_T), T)$	$\frac{d\langle C_A \rangle}{dt} = \frac{A}{V_R} < R_A(C_A, \phi(R_T), T) >$ - $\langle \mathbf{C_A} \rangle$: average concentration of species A - **t**: time - $\mathbf{V_R}$: reactor volume - **k(T)**: reaction rate constant - $\boldsymbol{\phi}(\mathbf{R_T})$: radiation field profile - $\mathbf{f}(\mathbf{C_A})$: species concentration profile

Conservation of Radiation

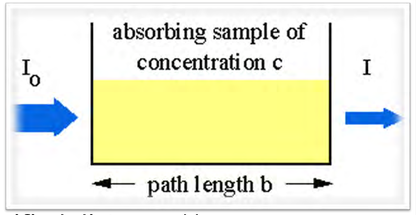
Assumptions	General Macroscopic Radiation Conservation Equation	Resulting Microscopic Radiation Equation
- Batch Reactor - Steady State - Isothermal - Isobaric - Monochromatic Light - Radiant Transport only in Radial Direction - Photon Reflection and Scattering are Neglected - Wall Reactions Only	$\frac{\partial}{\partial t}\int_V \eta_{\lambda\omega} d\lambda d\omega dV + \int_A \eta_{\lambda\omega}(c\vec{\Omega}) \cdot \vec{n} dA = \int_V (e_{\lambda\omega} - a_{\lambda\omega}) dV + \int_V J_{\lambda\omega,net} dV$ - $\boldsymbol{\eta_{\lambda\omega} d\lambda d\omega dV}$: Photon density function - $\boldsymbol{e_{\lambda\omega}}$ & $\boldsymbol{a_{\lambda\omega}}$: emission and absorption rates per units time and volume - $\vec{\boldsymbol{n}}$: normal vector - $\vec{\boldsymbol{\Omega}}$: directional vector - $\boldsymbol{J_{\lambda\omega,net}}$: net increase in photons per unites time and volume due to scattering phenomenon	$\phi(R_T) = I_0 e^{-\mu R_T}$ - $\boldsymbol{I_r}$: radiation field intensity at the photocatalyst surface - $\boldsymbol{I_0}$: initial intensity at the source. - $\boldsymbol{\mu}$: linear attenuation coefficient - $\boldsymbol{r}$: position at the photocatalytic surface

Discussion

Understanding the radiation field in the reactor is a vital component to developing a working model. This work is analogous to the findings by Cassano et al. (1984) regarding a photoreactor (as opposed to a photo*catalytic* reactor). As can be seen in the resulting equations, solving for the radiation field and the species concentration profiles all depend upon one quantity: the intensity of the radiation field (I_r). As shown in the diagram below, finding the magnitude of the radiation field allows us to first calculate the species reaction rate, $R_A(C_A, \phi(R_T), T)$, and finally the species mass concentration profile.

Species Mass	$\frac{d\langle C_A \rangle}{dt} = \frac{A}{V_R} < R_{A(}C_A, \phi(R_T), \mathrm{T}) >$	***(1)***
Reaction Rate.	$< R_{A(}C_A, \phi(R_T), \mathrm{T}) > = k\phi(R_T) < C_A >$	***(2)***
Radiation	$\phi(R_T) = I_0 e^{-\mu R_T}$	***(3)***

The equation found to represent the radiation field is a form of Beer-Lambert's Law [6]. This law tells us that as radiation with an initial intensity (I_0) enters a medium, the radiation intensity falls off exponentially as it moves a specified distance (r).



Conclusions and Future Work

We have used a volumetric(fluid phase) and area-averaging(catalyst phase) approach to obtain an upscaled model that holds promise for potential reactor design. The next steps will be to collect experimental data to validate the model. We plan to run experiments to obtain the final concentrations and the reaction constant(k_{app}). Both determinations will allow us to have an assessment of the model derived. We we will also work to confirm the accuracy of the upscaled species mass equation.

References

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