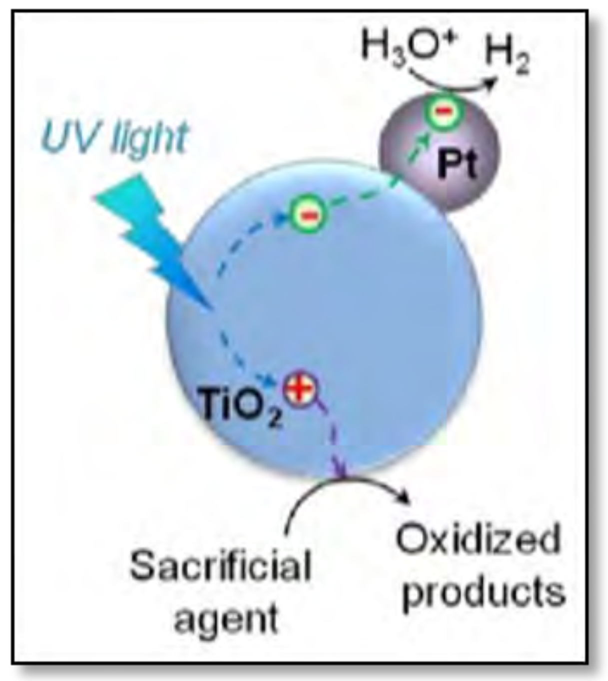
Modeling a Photocatalytic Reactor: Water Contaminant Degradation, Energy Production, and the Radiation Field

Sabrina Hurlock Buer[1], Pedro E. Arce[2], and Sunil Rawal[1]

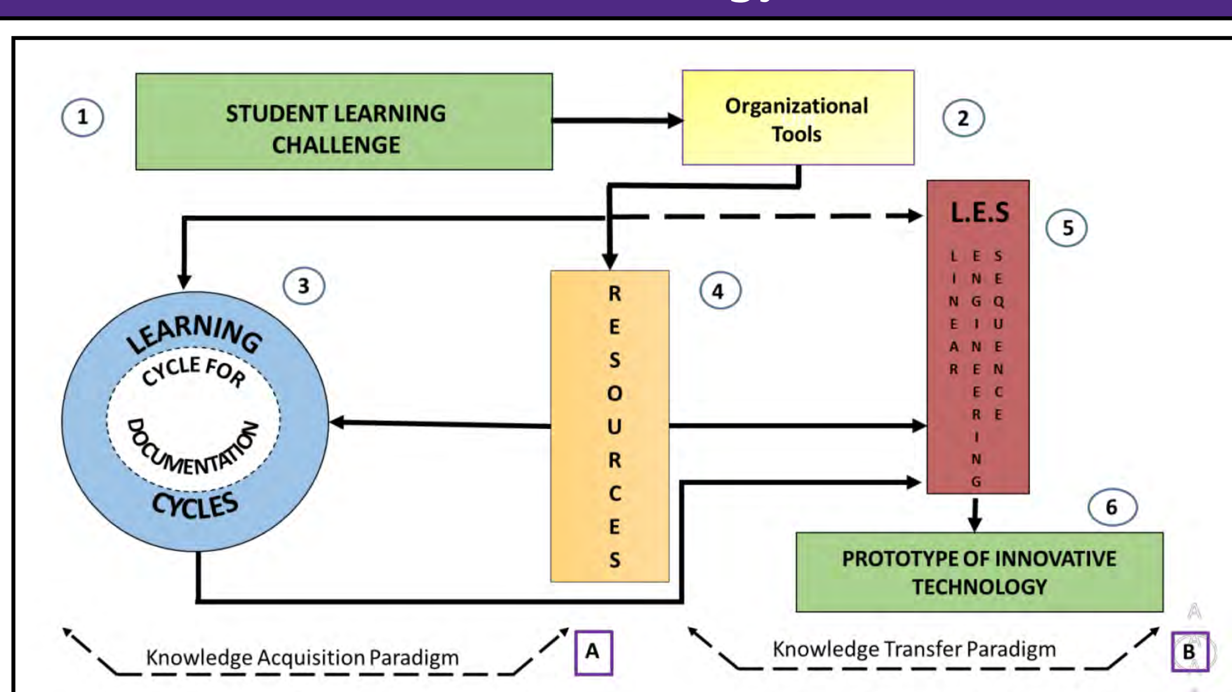
[1]Env. Sciences PhD Program, College of Interdisciplinary Studies, [2]Department of Chemical Engineering; Tennessee Technological University, Cookeville, TN

Motivation and Relevance of Research



As the amount of human and industrial waste in the environment increases, the need for more effective and efficient water treatment methods is higher than ever. Current wastewater treatment processes have been found to be ineffective against a growing number of contaminants, including pharmaceutical compounds. Coupled with the necessity of pharmaceutical-free water, energy sources that are easily produced, affordable, and environmentally-friendly are a growing societal need. This project will employ two photocatalytic approaches to address the issues of pharmaceutical degradation and energy production. The first method will utilize thin-film photocatalysis to achieve simultaneous contaminant degradation and hydrogen gas production as an energy source (pictured above [6]). The second method, and the focus of this poster, will model the photocatalytic reactor system (shown on the left [5]), allowing us to predict, optimize, and make more efficient the contaminant degradation and energy production processes. Additionally, this mathematical model is intended for future use as an upscaling mechanism to be used in wastewater treatment facilities.

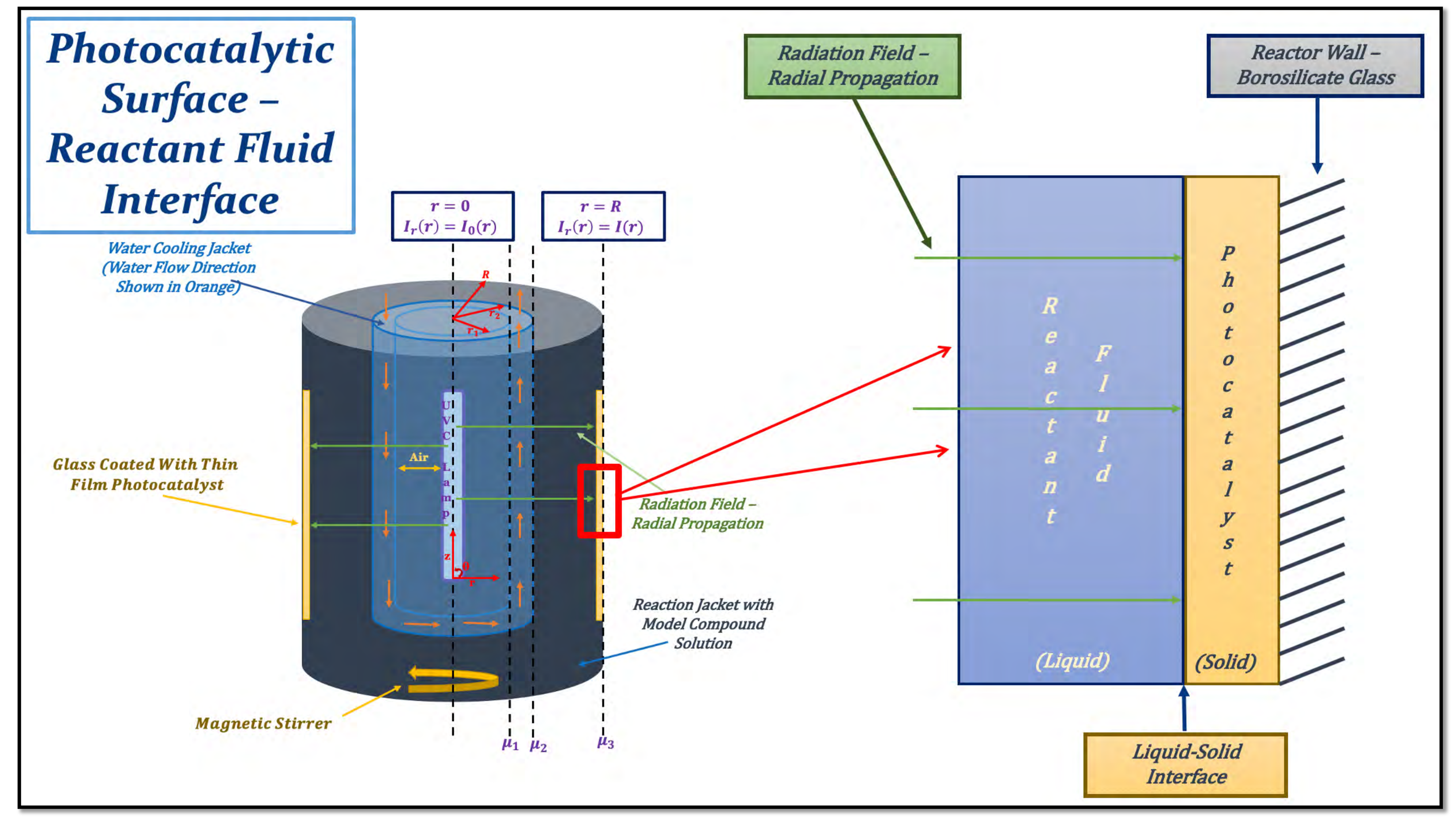
Methodology



The methodology for modeling the TTU photocatalytic reactor system is based on the Renaissance Foundry (see figure above) [3], the Soccer Ball Model [2], and the engineering upscaling approaches outlined in Arce et al., 2007. These combined works provide detailed procedures in regards to how to implement an effective modeling strategy, as well as the mathematical concepts needed (Divergence Theorem, Leibnitz Rule, area and volume averaging techniques, etc.) to both model the reactor and upscale the system for practical use.

Results

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	$\frac{\partial C_A}{\partial t} = \vec{\nabla} \cdot \vec{N_A} + R_A(C_A, T)$ - C_A: concentration of species A - t: time - N_A: total molar flux - R_A: reaction rate in fluid - T: temperature Interface Boundary Condition $\vec{N_A} \cdot \vec{N} = R_A(C_A, \phi(R_T), T)$	$\frac{d\langle C_A \rangle}{dt} = \frac{1}{V_R} k(T)\phi(R_T) f(C_A) A$ - $\langle C_A \rangle$: average concentration of species A - t: time - V_R: reactor volume - $k(T)$: reaction rate constant - $\phi(R_T)$: radiation field profile - $f(C_A)$: species concentration profile

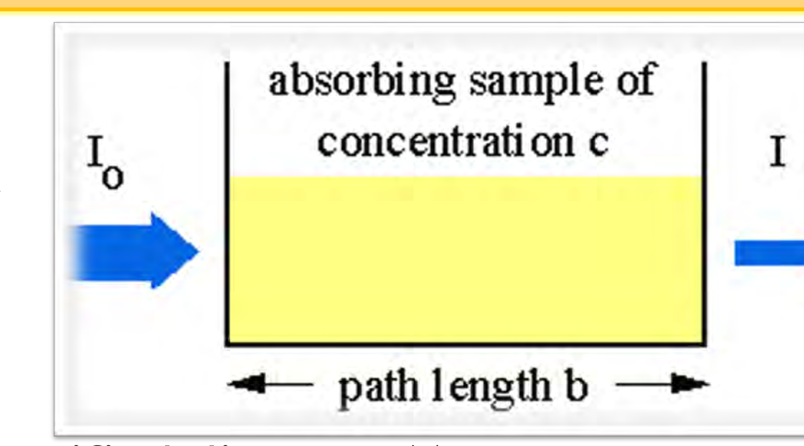
Conservation of Radiation

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	$\frac{\partial}{\partial t}\int_V \eta_{\lambda\omega} d\lambda d\omega dV + \int_A \eta_{\lambda\omega}(c\vec{\Omega}) \cdot \vec{n} dA = \int_V (e_{\lambda\omega} - a_{\lambda\omega}) dV + \int_V J_{\lambda\omega,net} dV$ - $\eta_{\lambda\omega} d\lambda d\omega dV$: Photon density function - $e_{\lambda\omega}$ & $a_{\lambda\omega}$: emission and absorption rates per units time and volume - $\vec{n}$: normal vector - $\vec{\Omega}$: directional vector - $J_{\lambda\omega,net}$: net increase in photons per unites time and volume due to scattering phenomenon	$\phi(R_T) = I_r = I_0 e^{-\mu r}$ - I_r: radiation field intensity at the photocatalyst surface - I_0: initial intensity at the source. - μ: linear attenuation coefficient - 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	$\frac{d\langle C_A \rangle}{dt} = \frac{1}{V_R} k(T)\phi(R_T) f(C_A) A$	**(1)**
Reaction Rate	$R_A(C_A, \phi(R_T), T) = kI_r C_A$	**(2)**
Radiation	$\phi(R_T) = I_r = I_0 e^{-\mu r}$	**(3)**



The equation found to represent the radiation field is a form of Beer-Lambert's Law [7]. 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

The preliminary results of this reactor model are promising. The future of this model depends upon finding an expression for the average species concentration, $\langle C_A \rangle$. Additionally, the linear attenuation coefficients (μ_1, μ_2, and μ_3), as shown in the TTU reactor schematic, must be determined for each region as the radiation moves through the system toward the photocatalytic surface. These values will allow us to calculate the reaction rate and species concentration profile, allowing for eventual reactor scale-up.

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