Investigating the Impact of Gas Fraction on Photon Transport in Taylor-Flow Reactors

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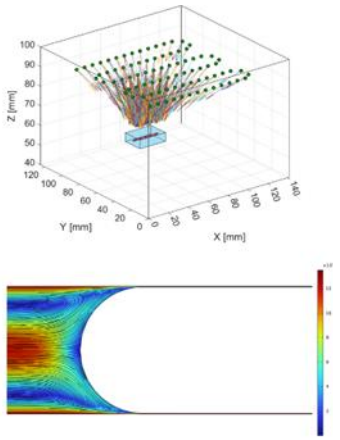

Taylor flow is well-known for its benefits in microreactors, such as enhanced mixing, improved mass transfer, scalability, and reaction intensification. However, the impact of Taylor flow on light-driven reactions is not fully understood. This study investigates how Taylor flow affects photon transport, specifically examining the influence of varying gas fractions on photon behavior in confined microscale environments. Applying ray-tracing simulations and Computational Fluid Dynamics (CFD), this work aims to analyze the interaction between gas fraction and photon transport. Our findings emphasize the crucial role of well-designed flow systems in achieving efficient light-driven reactions in microreactors and lab-on-a-chip devices, highlighting the need to consider both fluid dynamics and photon behavior.

Introduction

Taylor flow is well-studied in fluid dynamics for its effects on fluid mixing and heat and mass transport. However, its influence on light transport within microchannels is still not fully understood. Understanding how Taylor flow affects photon transport is crucial for optimizing reaction efficiency.

To address this, CFD and ray-tracing simulations offer valuable insights. CFD analyzes fluid behavior, aiding in microreactor design without compromising performance. Ray-tracing simulations are essential for understanding light-fluid interactions in microreactors, particularly in light-driven reactions.

This study examines the impact of gas fraction variations on photon transfer in a gas-liquid flow using an in-house ray-tracing code developed by Roibu et al. (2023) [1], alongside CFD software. The primary objective of this work is to introduce a methodology suitable for elucidating various aspects of photocatalytic systems with the gas-liquid Taylor flow pattern.

Material and Methods

The interference of Taylor bubbles on photon transfer was evaluated using the light-dependent photooxidation of 9,10-dimethylanthracene (DMA) as the benchmark reaction. This allowed an analysis of the interference of gas fractions in the reaction rate of the system. All simulations were conducted with air as the dispersed phase and ethanol as the continuous phase.

The ray-tracing model analyzed light interactions in the microreactor, tracking ray reflection, refraction, and total internal reflection at media interfaces. It used Snell's law and Fresnel equations to determine ray direction and intensity, while attenuation followed the Beer-Lambert-Bouguer law [1]. The system was illuminated by an LED board with forward current I_F = 1.77 mA/LED, and the output collected was the power in mW absorbed in the liquid phase.

By simulating gas fractions of 0.25, 0.5, and 0.75 using a ray-tracing simulation code, the power reaching the liquid phase of the system was determined. This information was then incorporated into the light-dependent kinetics in the CFD simulation. Three kinetics were developed, considering β_G equal to 0.25, 0.5, and 0.75, based on the experimental study by Roibu et al. (2023) [1]. The pseudo-first-order specific rate constant was then determined according to Equation 1 [2]:

$$-\ln(1 - X_i) = kt \quad (1)$$

Plots of $-\ln(1 - X_i)$ versus t were created for each β_G. An equation representing the relation between the rate constant and the powers was then created. After inserting the power acquired in the ray-tracing simulations into the kinetics, CFD simulations were carried out to observe the influence of fluid dynamics on the conversion.

The microchannel's gas-liquid Taylor flow was simulated within the context of the bubble frame of

reference. This approach maintains the gas bubble stationary while the wall is set in motion. The flow behavior is simulated within a unit cell, and the length of this unit cell was set to simulate 2 bubbles and 3 slugs. The size of the bubble, slug, and thickness film (among others) are calculated through correlations.

The liquid film thickness was calculated from the Bretherton correlation [3]:

$$\frac{\delta}{D} = \frac{1}{2} \cdot 0.643 \cdot (3 \cdot Ca_D)^{2/3} \quad (2)$$

where Ca is the Capillary number, and D is the diameter of the microchannel.

Following, the bubble length was calculated [4]:

$$L_B = D \cdot [1.637 \cdot \varepsilon_G^{0.107} \cdot (1 - \varepsilon_G)^{-1.05} \cdot Re^{-0.075} \cdot Ca^{-0.0687}] \quad (3)$$

where ε_G is the gas fraction and Re is the Reynolds number.

The slug length was then calculated as follows [4]:

$$L_L = D \cdot [1.637 \cdot \varepsilon_G^{-0.893} \cdot (1 - \varepsilon_G)^{-0.05} \cdot Re^{-0.075} \cdot Ca^{-0.0687}] \quad (4)$$

Results and Discussion

The mathematical modeling demonstrated a good response when compared to experimental findings (Figure 1). As expected, higher gas fractions were associated with the generation of larger bubbles and smaller slugs within the system.

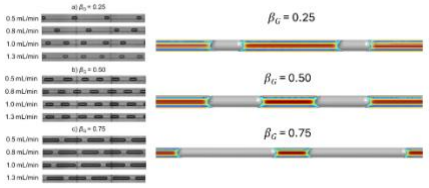

Figure 1. Visual representation of both experimental data and simulated results.

The analysis presented herein has focused on a single residence time to examine the influence of gas fraction. This approach allowed us to observe a consistent pattern in the ray-tracing simulations: as the gas fraction increased, so did the power absorbed by the liquid phase. This observation was further supported by Computational Fluid Dynamics (CFD) simulations, where higher gas fractions corresponded to increased conversion rates under identical conditions (Table 1).

Table 1. System response under varying gas fractions.

β_G	L_L(mm)	L_B(mm)	δ (μm)	Pabs (mW)	X_{DMA}(%)
0.25	7.20	2.40	9.37	0.13	1.90
0.50	3.95	3.95	9.36	0.14	3.43
0.75	2.85	8.55	9.40	0.18	6.45

* the conversion (X_{DMA}) is considering a single cell.

Despite being larger, the bubbles seemed to contribute to greater absorption in the liquid phase, even when the overall absorption rates in the reactor were relatively low. This could be explained by the fact that larger bubbles create longer paths of interaction within the liquid phase, and also because they interfere in the light reflection and refraction.

This phenomenon highlights the interesting interplay between gas-liquid dynamics and light absorption, emphasizing the necessity of considering multiple factors to optimize reactor performance effectively. Additionally, the analysis revealed that variations in film thickness did not seem to have a significant impact on the power absorbed by the liquid. This observation suggests that factors such as gas bubbles and slug size could play more dominant roles in determining absorption rates within the system.

Conclusions

The method proved successful in examining photochemical reactions in Taylor flow. Further investigation is necessary to identify the factors that correlate bubble size to light absorption in the liquid phase. Additionally, future studies should consider parameters like residence time, microchannel diameter, and liquid/gas velocities, among others.

Acknowledgments

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