

“PAPER FOR THE YOUNG SCIENTIST AWARD”**Controlling Thermocapillary Droplet Migration via Interfacial Reactions**

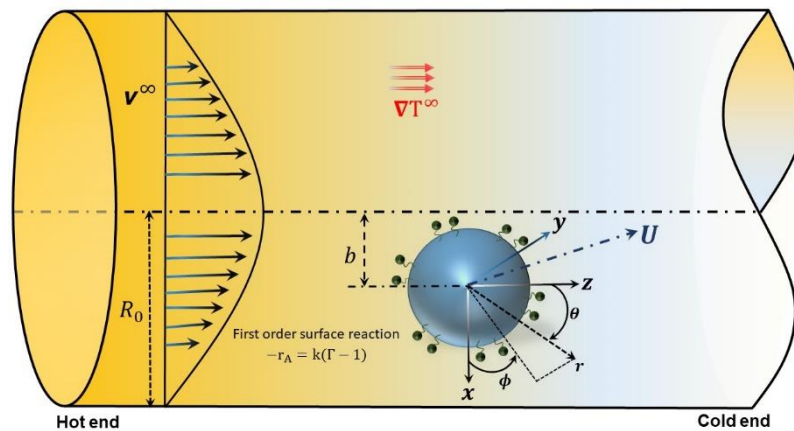
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1. INTRODUCTION & OBJECTIVE

Living organisms exhibit dynamic functionalities driven by complex chemical reactions. Interfacial reactions lead to phenomena like convection, chemical gardens, and self-propelled droplets, which reduce surface tension by dissolving surfactants [1]. Studies on droplet motion show that surfactant-induced Marangoni stresses influence migration velocities. Hanna & Vlahovska [2] observed cross-stream migration in Poiseuille flow at large surface Péclet number (Pe_s) limits, while Pak et al. [3] explored similar effects under small Pe_s limits. Sharanya et al. [4] and Basak et al. [5] further examined the role of nonlinear interfacial tension and thermal dipoles in controlling migration direction.

In our work, we model a droplet undergoing a first-order interfacial reaction that alters surfactant activity, simulating self-propulsion as shown by Thutupalli et al. [6]. The droplet, influenced by external Poiseuille flow and thermal gradients, exhibits migration behaviors due to differences in its physical properties from the surrounding medium. We propose a novel method for capturing and transporting droplets hydrodynamically, with potential applications in drug delivery and biomedicine.

2. MATHEMATICAL MODELLING

Consider the surfactant-laden droplet of radius a is suspended in a Poiseuille flow. This flow experiences an external thermal gradient ∇T_∞ . Assuming negligible fluid inertia and thermal convection, the non-dimensional mass, momentum and energy equation follows,

$$\nabla \cdot \mathbf{u}^j = 0, \quad -\nabla p^j + \frac{\mu^j}{\mu^e} \Delta \mathbf{u}^j = 0, \quad \Delta T^j = 0, \quad \text{for } j = i, e.$$

The superscripts ‘ i, e ’ denotes the flow variables internal/external to the droplet. The surfactant concentration over droplet interface ($r = 1$) satisfies,

$$Pe_s \nabla \cdot (\Gamma \mathbf{u}_s) + k(\Gamma - 1) = \Delta_s \Gamma.$$

Here, Γ is the surfactant concentration, \mathbf{u}_s is the surface velocity and k is the non-dimensional reaction coefficient (often know as Thiele Modulus). The interface conditions ($r = 1$) are as follows:

1. $\mathbf{u}^e \cdot \mathbf{n} = 0 = \mathbf{u}^i \cdot \mathbf{n},$
2. $\mathbf{u}^e \cdot \mathbf{t} = \mathbf{u}^i \cdot \mathbf{t},$
3. $\boldsymbol{\tau}^e \cdot \mathbf{n} \cdot \mathbf{t} - \boldsymbol{\mu} \boldsymbol{\tau}^i \cdot \mathbf{n} \cdot \mathbf{t} = \nabla_s (Ma_T T^e + Ma_\Gamma \Gamma) \cdot \mathbf{t},$
4. $T^e = T^i,$
5. $\nabla T^e \cdot \mathbf{n} = \kappa \nabla T^i \cdot \mathbf{n},$

where Ma_T and Ma_Γ are the Marangoni numbers. Also far from the droplet as $r \rightarrow \infty$, $\mathbf{u}^e \rightarrow \mathbf{v}^\infty - \mathbf{U}$, $p^e \rightarrow p^\infty$, $T^e \rightarrow T^\infty$, and internal to the droplet as $r \rightarrow 0$, \mathbf{u}^i , p^i and T^i are bounded. Here \mathbf{U} is the unknown migration velocity of the droplet and \mathbf{v}^∞ , p^∞ and T^∞ are known from the applied far-field Poiseuille flow and constant thermal gradient conditions.

We first solve the thermal energy equations considering the interface and boundary conditions. By employing asymptotic regular perturbation in terms of small Pe_s , we simultaneously analyze the surfactant concentration and velocity fields. The solenoidal decomposition approach is employed to solve the Stokes flow equations at every order of perturbation. Detailed procedures for determining the drag and the corresponding migration velocity of the droplet similar to Basak et al. [5].

3. RESULTS & HIGHLIGHTS OF IMPOINTANT POINTS

Our results indicate that the droplet undergoes both streamwise and cross-stream migration. The thermal Marangoni number accelerates migration, while the surfactant-induced Marangoni number slows it down. Surface chemical reactions primarily influence streamwise migration velocity in the first order of Pe_s , and cross-stream migration in the second order. We analyzed the trade-off between the surface reaction parameter and Marangoni number, identifying zones where migration velocity is optimized. Additionally, we calculated the critical Marangoni number at which the droplet changes its migration direction, noting that it increases with higher reaction rates. This study highlights the significance of surfactant-reaction effects on thermocapillary droplet motion, with implications for control applications. Our analytical findings offer essential benchmarks for future computational studies in droplet dynamics.

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