ABSTRACT

The field of microfluidics and nanofluidics are witnessing a plethora of non-trivial interfacial behaviour in fluid flows due to unprecedented advancements in experimental and computational resources in recent years. While the particulars of these eccentric interfacial features continue to induce unanswered inquiries, they simultaneously present an array of auspicious prospects for ground-breaking developments in fields such as lab-on-chip technology, biomedical devices, microelectronic cooling, and smart surface engineering, among others. At microscale flow systems, surface forces dominate volumetric forces, leading to complicated variations in diverse flow properties making the interfacial effects crucial to decide the flow outcomes. Furthermore, when the characteristic length is reduced to the nanometer range and approaches the molecular scale, molecular interactions may become prevailing, possibly challenging the continuum hypothesis.

The present dissertation aims to offer critical insights into understanding the non-trivial interfacial links between bulk and interfaces in micro and nanoscale flow systems with theoretical and numerical approaches. This thesis begins with the study where we attempt to delve deeper into the dynamic flow conditions in nanofluidic channels with axially varying cross sections where upstream events may have significant influences on the flow behaviour. Without relying on comprehensive molecular dynamics simulations, this study presents advancements in hybrid molecular-continuum simulations with the ability to predict water transport through converging nanopores. Subsequently, we recognise a remarkable flow rectification behaviour in micro-nanochannel junctions where the slip coefficient may have capabilities to demarcate various flow regimes within such systems. Such systems may have wide applicability in applications like water desalination, membrane separation etc. Furthermore, the flow characteristics in micro and nanochannels can be significantly influenced by the physical and chemical qualities of the surface and we attempt to study the interplay between physical properties, such as surface roughness, and chemical traits, such as wettability, leading to a diverse range of distinct flow phenomena. When considering the ramifications of significant interfacial effects in multiphase flow systems, it is imperative to comprehend the influence of these effects on the distribution of phases, pressure drops, and heat transfer. This thesis introduces a comprehensive paradigm for characterizing the immediate behaviour of droplets after their impact on a surface using simplified lumped parameters that are similar to those employed in basic harmonic oscillators. Additionally, the process of droplet evolution and breakage following deformation within microconfinement is a significant phenomenon that bears a resemblance to the water management system in a Proton Exchange Membrane (PEM) fuel cell. In this study, we present a novel micro-patterned surface design that aims to enhance the efficiency of water removal from Proton Exchange Membrane Fuel Cells (PEMFC). In summary, from the manipulation of fluid slippage at the interface between a liquid and a solid within nanochannels to the exact control of the shape and stability of the interface in multiphase flows, these examples exemplify the wide range of outcomes resulting from the diverse interfacial effects that may serve purposes in a wide gamut of applications such as water desalination, drug delivery, microelectronic cooling, point-of-care devices, energy conversion systems, PEM fuel cells among others.

Keywords: Microfluidics, nanofluidics, interfacial effects, wettability, slip, roughness, bulk, interfaces, multiphase flow, textured surface.