Preface

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I would like to start the preface to the Special Issue on Multiscale Transport Phenomena by giving a brief account of the history of this still very young research field. The reports on multiscale simulations of transport phenomena (momentum, heat, and mass transfer) started to appear in the literature in the late 1990s, and their count is still in the dozens, not hundreds. The first attempts in the field were undertaken by the chemical engineers, who have always been interested in reconciling the disparity of characteristic length and time scales in simulations of heterogeneous transport-reaction systems. In a traditional approach, the reactor scale (global) transport processes and the interfacial (local) processes (e.g., surface catalytic reactions or growth of deposits/thin films) have been treated as only one-way interactions, thereby decoupling the macroscale (reactor level) and microscale (interface level) processes. It was an important realization when the importance of accounting for multiscale (macro-to-micro and micro-to-macro scale) interactions for correct prediction of chemical vapor deposition (CVD) process was demonstrated, and several algorithms for handling the multiscale paradigm were proposed. Among the most notable examples, Vlachos [1,2] proposed the hybrid MIH algorithm employing the domain decomposition method based on partitioning the system into two overlapping subdomains (gas and surface) of different scales, and subsequent use of Monte-Carlo simulations for the surface processes to supply the boundary conditions for the continuous mass and momentum transport models in the adjacent boundary layer. The application of the MIH algorithm was restricted to isothermal systems and required significant computer power, thereby reducing the applicability of the method for practical engineering calculations. Jensen's group at MIT performed multiscale modeling of thin-film growth [3], chemical vapor deposition [4], and heterogeneous chemical reactors [5]. In Jensen's approach, the macro (continuum) and micro (discrete particle) transport regimes were linked by an effective reactivity function (ε) to integrate the effects of multiscale surface heterogeneity and microscale transport resistance. Calculations of an effective reactivity function were accomplished by a hybrid ballistic transport, the Monte Carlo method, while the Galerkin method employing standard bases, such as Fourier series and finite elements, was used to simulate multiscale fluid flow and thermal and concentration fields. Finally, Fedorov and Viskanta have developed and experimentally validated a hybrid theoretical methodology for the time efficient dynamic simulations of heterogeneous gas separation systems [6–9]. Their approach combined the continuous flow, conjugate heat and

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mass transfer models with the simplified local density (SLD) statistical mechanics model for adsorption equilibrium within a unified computational framework [6]. Both no-slip (continuous regime [7,8]) and slip (Knudsen semicontinuous regime [9]) flows have been considered, depending upon the dimensions of the system. The main advantage of the latter approach was its practicality for use as an engineering analysis tool, owing to fundamentally sound, yet computationally affordable semianalytical treatment of surface physicochemical interactions. It was also shown that the interactions between heat and mass transport (on the millimeter and micrometer scale) and adsorption/desorption (on the nanometer scale) significantly influence the overall dynamics of the system, and this influence manifests itself in a strongly nonlinear fashion. Comparison of the measured and predicted transient temperature and concentration uptakes unambiguously proved the vital importance of careful accounting for multiscale interactions (i.e., the information exchange between the micro- to the macroscales).

As we entered the twenty-first century, the micro- and nanotechnologies have quickly risen to a dominant position on the nation's and the world's research agenda. As the sizes of the devices shrink, new phenomena emerge that can no longer be adequately described using conventional transport theories in the limit of the continuous description of the medium. This provided a strong impetus for the development of new physical models and computational algorithms that could be used to understand the fluid flow and heat and mass transport across the length scales spanning several orders of magnitude. Thus, an interest in multiscale computation of transport phenomena is on a rise again owing its fundamental importance to behavior prediction and design of micro/nano systems. This special issue is a compilation of original papers and review articles on multiscale transport phenomena by the current leaders in this emerging field. To stimulate future research, the issue provides a balanced combination of the broad prospective and the in-depth coverage on the current state of the art and the remaining challenges. All contributions are invited and cover both the key subdisciplines of transport phenomena (e.g., gas flow in confined geometries, heat conduction in submicron structures and semiconductors, surface and bulk diffusion of chemical species, transport in porous media) and multiphysics problems (e.g., multiscale radiation-turbulence interactions and multiscale electrochemistry-species transport interactions in porous media). In addition, all papers have a clear emphasis on very important emerging applications, ranging from thermal management of micro/nanoelectronics to fuel cells, to bioanalytical microfluidic lab-on-a-chip devices. In conclusion, I hope that with the high-quality contributions from the leading researchers in the field of multiscale computations of transport phenomena, this special issue of IJMCE will become a valuable guide for future research in this emerging field.

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