501a Hierarchical Modeling of Integrated Microdevices for Hydrogen Production

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With significant developments in microelectronics, telecommunication, micro-electro mechanical systems (MEMS) and related technologies, newer and more efficient sources of portable power generation are being developed for both civilian and military applications. Hydrogen-based power sources, such as the PEM fuel cells, are envisioned as the candidates for the 1 – 100 W applications. One of the main challenges is the reliable and on-demand generation of CO-free hydrogen, given the inability of the current hydrogen storage methods to meet the practical requirements of safety, weight and cost. Coupled microreactors that integrate endothermic reforming or thermal decomposition reactions with exothermic combustion reactions are being developed for this purpose.

In this paper, we present a theoretical study on hydrogen generation in multifunctional microreactors by considering a range of reactor models of increasing complexity. Our overall objective is to predict suitable materials, flow configurations, mixing patterns, and operating conditions that improve efficiency of small scale systems. While two-dimensional (2D) computational fluid dynamics (CFD) models are able to provide an in-depth understanding about the operational characteristics of an integrated microreactor, they are computationally too demanding for determining stability limits and optimal operating regimes. Herein, we develop a hierarchical modeling scheme ranging from simple energy and material balances to 2D CFD in order to assess the level of sophistication needed and develop systematic strategies that enable simple reactor models to be accurate by suitable parameterization from more complex models. Based on the scaling analysis of the various processes in the microreactor, a gauge of the predictive capabilities of the various models can be obtained. Identification of the relevant parameter space based on simple models can guide us to the right operating regime, which is further refined using higher level, but computationally more demanding CFD models. We also investigate whether the hierarchical approach can be used to determine the existence of interesting features, such as Hopf bifurcation, that lead to instabilities and failure of microdevices. The approach will be demonstrated for ammonia decomposition on Ru catalyst, which produces hydrogen, coupled with fossil fuel combustion. Both simple and complex reaction mechanisms will be discussed.