MicroChemical Systems for Direct Fluorination of Aromatics

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Aromatic compounds containing one or two fluorine ring substituents are important intermediates used in the synthesis of pharmaceuticals, crop protection agents, and as monomers for manufacturing high-performance aromatic polymers. A one-step process to selectively fluorinate a potentially wide range of aromatic compounds would be by reacting the aromatic with elemental fluorine. The direct fluorination of aromatics, however, is a highly exothermic process difficult to control on a large scale. Heat management is essential to achieve good reaction selectivity.

Over the last decade, the fabrication techniques originally developed for the microelectronics industry have expanded to the fabrication of microfabricated chemical reactors. Microfabricated reactors, with feature sizes in the micron to hundreds of micron range, are inherently safe. The large surface-to-volume ratios available in these systems translate into high heat and mass transfer rates. In addition, microfabrication enables the design of novel multiphase reactors. It is also possible to integrate temperature sensors and detection systems. Microfabricated reactors thus offer unique opportunities to perform direct fluorination reactions under more aggressive conditions than in bench top systems while achieving good heat control.

We are developing an integrated microfabricated chemical system that enables selective and safe direct fluorination of aromatic compounds. The reactor is built in silicon, capped with Pyrex, and coated with protective silicon oxide and nickel films (Figure 42). The first reactor design consists of two reaction channels with triangular cross-section. This type of geometry provides a large gas-liquid interfacial area and facilitates the deposition of the nickel films. Liquid and gas reactants flow cocurrently through the channels. The selective direct fluorination of toluene as model chemistry is successfully demonstrated at room temperature. Conversion and product distribution are investigated as a function of the operating conditions: solvent, substrate concentration, and number of fluorine equivalents. The direct fluorination of heteroaromatic compounds is under investigation. Mass and heat transfer models are used to understand and optimize the performance of the reactor.

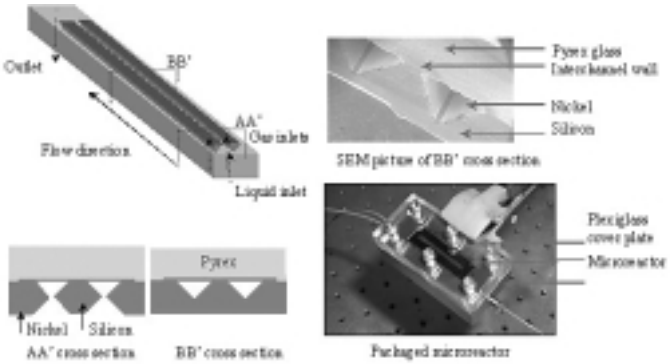

Fig. 42: Microreactor for direct fluorination – nickel coated channels (left) – packaged device (right)