268c Analytical Method of Lines for Predicting Multiple and Asymmetric Steady States in Catalytic Monolith Reactors - Diffusive Transport

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Monolith reactors are suitable for carrying out fast reactions in applications where space is a constraint. Important examples are car exhausts, fuel cell reforming, oxidation of volatile organic compounds (VOCs) and gas-liquid reactions. Advantages of monoliths include, absence of a need for filtering, a high geometrical surface area, safer operations, easier scale up and reduced misdistribution problems. Modeling transport in catalytic monolith reactors is still an active area of research1-3 because of the existence of multiple and asymmetric steady states. A rigorous numerical solution for the models governing these reactors are not efficient because [1] There exists multiple, meaningful solutions [2] Initial guess needs to be good [3] Number of node points needs to be very high because of possible steep gradients in the radial direction.

We have developed a novel efficient analytical method of lines (AMOL) approach for simulating transport in monolith reactors. The AMOL method involves converting a given elliptic PDE (x,y) to N 2nd order Ordinary differential equations in one of the independent space variables (say, y). The derivatives in x are approximated using finite differences accurate to order h2. The resulting system of coupled ordinary differential equations in y is integrated using the matrix methods to get a closed-form solution in y and the system parameters.4,5

The advantages and disadvantages of the proposed method in predicting multiple steady states for various modes of transport will be discussed.

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