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MODELING FIXED BED CHEMICAL REACTORS WITH HIGH HEAT RELEASE

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Abstract. In this study, a mathematical model was developed to simulate the steady-state and dynamic behaviors of a fixed-bed reactor used for a highly exothermic hydrotreating process of a cracked naphtha. A second order, backward finite difference method was used for the discretization of the PDEs to overcome the stiffness of the equations in the axial direction, which was caused by the reaction term, coupled with the high heat release due to hydrogenation reactions. The model successfully simulated the temperature and conversion profiles in the reactor under steady-state operation. It also qualitatively captured the different start-up dynamic behaviors of a longer and a shorter catalyst bed reactor, the creeping “hot spot” during start-up, and the reactor temperature responses to a step-change in hydrogen flow rate.
Keywords. Fixed bed reactors, modeling and simulation, partial differential equations, finite difference
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1 Introduction

Fixed-bed reactors, in which gases flow through cylindrical beds packed with catalyst particles to undergo chemical reactions, are widely used in chemical, petrochemical and petroleum refining processes (see [2], [4], [6]). The design and performance optimizations of these commercial processes rely, to a large extent, on successful reactor simulation using mathematical models based on mass, heat and momentum balances (see [2], [13]). Such reactor models usually consist of a set of partial/ordinary differential equations (PDEs/ODEs) with well-defined initial and boundary conditions. However if a large amount of heat is released due to chemical reactions, the numerical computation of these PDEs/ODEs could become difficult due to the stiffness of the equations, which is caused by the reaction term (reaction rate changes exponentially with reaction temperature) coupled with the strong heat release. Consequently, serious challenges could be expected in process design, control and operation.

This paper discusses the modeling and simulation of dynamic and steady-state behaviors of a catalytic fixed-bed reactor used for hydrotreating of a partially stabilized coker naphtha – a highly exothermic petroleum refining process. The