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Abstract

Adsorptive reactors(AR), in which an adsorptive functionality is incorporated into the catalytic reactors, offer enhanced performance over their conventional counterparts due to the effective manipulation of concentration and temperature profiles. The operation of these attractive reactors is, however, inherently unsteady state, complicating the design and operation of such sorption-enhanced processes. In order to capture, comprehend and capitalize upon the rich dynamic texture of adsorptive reactors, it is necessary to employ cyclic steady state algorithms describing the entire reaction-adsorption/desorption cycle. The stability of this cyclic steady state is of great importance for the design and operation of adsorptive reactors. In this paper, the cyclic steady state of previously proposed novel adsorptive reactor designs has been calculated and then optimized to give maximum space-time yields. The results obtained revealed unambiguously that an improvement potential of up to multifold level could be attained under the optimized cyclic steady state conditions. This additional improvement resulted from the reduction of the regeneration time well below the reaction-adsorption time, which means, in turn, more space-time yield.

Keywords: Adsorptive reactors; Multifunctional reactors; Cyclic steady state; Claus reaction; Deacon reaction

1. Introduction

Cyclic fixed bed processes are operated, in most cases, by repeating a sequence of predefined steps continuously until these cycles reach, or asymptotically approach, a condition, at which any state of the bed at any point in the cycle is identical to the previous cycle. This condition is known as a periodic state or cyclic steady state. Determining and optimizing the cyclic steady state receive significant technological interest for developing new cyclic processes or improving already existing ones. Pressure swing adsorption (PSA), temperature swing adsorption (TSA), and reverse flow reactors are common examples of such processes. With no exception to the abovementioned inherently cyclic nature, adsorptive reactors, or sorption enhanced processes as also widely known in the literature, represent a promising and upcoming technology for several important and equilibrium-limited processes applied in industry. The cyclic steady state behavior and process cycle design of adsorptive reactors have been extensively studied in the literature. For instance, the working group of Rodrigues in Portugal designed three-, four-, and five-step cycle operation of adsorptive reactors, the former for dehydrogenation of ethane to ethylene [1] and the latter ones for steam-methane reforming [2,3]. For all developed cycle designs, the periodic state was determined, for which an improved performance over the conventional processes was reported. A similar conclusion has been also made by Rawadieh and Gomes [4] for a five-step cyclic adsorptive steam reforming reactor. With five cyclic steps design including reaction-adsorption, depressurization, purge I and II, and pressurization, Hufton *et al*. [5] reported about 200% process improvement over the conventional process.

Mathematical modeling and optimization offer an economical tool for investigating a wide range of process alternatives and configurations. Nevertheless, improved calculating algorithms and optimizing routines are necessary to accelerate the solution process over the extremely time-consuming conventional techniques. For example, cyclic steady states are typically determined by the so-called successive substitution method, in which the process is simulated one cycle after another until convergence to the cyclic state is reached. This method is computationally infeasible for complex systems. Several approaches to speed up the convergence and subsequently reach the solution have been successfully proposed and implemented. Gorbach *et al*. [6] introduced a general method to derive