

Simulation of the catalyzed isotopic exchange between hydrogen and water in a trickle bed reactor



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HIGHLIGHTS

- Limiting step of overall isotopic exchange alters near bottom of the reactor.
- Molar flow rate ratio in feed and dilution ratio in catalyst bed are optimized.
- Hydrogen humidifying affects deuterium removal in hydrogen.

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ABSTRACT

The catalytic exchange column of countercurrent trickle bed for deuterium removal from hydrogen is simulated based on experimental results along with established reaction and mass transfer models, accounting for the humidification of hydrogen in a catalyst bed filled with platinum/styrene-divinylbenzene copolymer pellets and Dixon rings. Relative deviations of less than 30% are achieved between the experimental and the simulated HD molar fractions at the column outlet. Simulation results indicate that hydrogen humidification exerts a noticeable influence on gas and liquid phase flow rates, leading to an overestimated removal percentage of deuterium when such flow rate variances are neglected. Rate limiting step for the overall gas-liquid isotopic exchange is discussed. Finally, the operation conditions are optimized using the developed model.

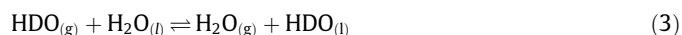
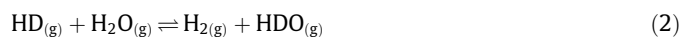
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1. Introduction

Catalyzed isotopic exchange between hydrogen and water is an effective method for separating hydrogen isotopes during waste water treatment of future fusion reactors and heavy water upgrading of fission reactors (Alekseev et al., 2002; Ionita et al., 2015; Vasyanina et al., 2008). Some matured methods such as liquid phase catalytic exchange (LPCE) and combined electrolysis and catalytic exchange (CECE) have been recognized as prospective tritiated water treatment techniques for the International Thermonuclear Experimental Reactor (ITER) (Ana et al., 2009; Ionita et al., 2015). Alekseev et al. (2011) produced highly purified heavy water and deuterium gas in a pilot CECE plant for heavy water upgrading and detritiation.

The overall process of catalyzed isotopic exchange between deuterated hydrogen and water (Eq. (1)) can be divided into two

steps: catalytic exchange in gas phase (Eq. (2)) and gas-liquid mass transfer of HDO (Eq. (3)) (Ovcharov et al., 2009).



Noble metals presented high catalytic activities for the isotopic exchanges merely in gas phase, which therefore made the process for gas-liquid isotopic exchange complicated (Kumar et al., 2013; Ye et al., 2013). Stevens (1972) designed the first hydrophobic catalyst for combining gas-liquid mass transfer and catalytic exchange in a catalytic exchange column of a countercurrent flow trickle bed (Kumar et al., 2013). Gas-liquid mass transfer in catalyst bed was enhanced by mixing hydrophilic packing with hydrophobic catalyst (Ye et al., 2014).

Simulation of the catalytic exchange column, which is the main facility of LPCE and CECE, is important for the design and optimiza-

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