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Autothermal Operation in a Simulated Moving Bed Reactor

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Highlights

- Experimental and model based investigation of Simulated Moving Bed Reactor
- Estimation of reaction kinetics using individual adsorption isotherm measurements
- Identification of operation window and experimental evaluation

1. Introduction

The purification of industrial volatile organic compound (VOC) exhaust streams requires special attention. To fulfill the emission standards in an efficient way, autothermal process using the exothermicity of the oxidation reactions to preheat the diluted feeds were investigated in the last decades [1]. Inspired by separation processes, which exploit a countercurrent movement between fluid and solid phases, a promising innovative concept is the Simulated Moving Bed Reactor (SMBR) [2-4].

The concept requires an adiabatic reactor cascade of at least two reactor segments (Fig. 1a, $N_{seg} \geq 2$). If cold feed gas enters a first hot reactor segment I the reactants are heated-up to the ignition temperature T_{ign} and the desired total oxidation proceeds. The formed exothermal reaction front moves in the direction of the flow. After passing completely the segment I, the feed and outlet port position are shifted in the direction of the flow following the temperature and reaction fronts. Thus, the formerly cold first segment is switched at the end of the reactor cascade and the hot exhaust gas can heat-up it up again. This periodical process attempts to trap a self-sustained exothermic front and, thus, allows an autothermal process operation. Two fronts traveling with different speed are formed, the exothermal reaction front and the thermal front (u_R and u_T in Fig. 1b), respectively.

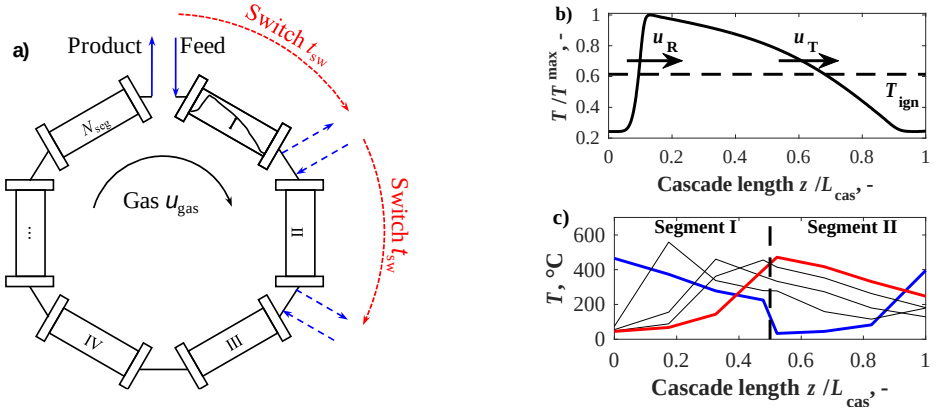

Figure 1. (a) Principle of the Simulated Moving Bed Reactor: A periodically operated reactor cascade of N_{seg} catalytic fixed beds based on switching simultaneously in- and outlet port positions in the gas flow direction, (b) the modeled temperature profile including the illustrated traveling exothermal reaction (u_R) and temperature (u_T) fronts in the middle of a switching period, (c) experimental observed temperature profiles in a two reactor segment cascade (feed on segment I), snapshots within one switching period

2. Methods

To predict cyclic stable ignited conditions of the SMBR several issues have to be considered. To reduce computational efforts, model based predictions using a simplified SMBR model were presented by Zahn et al. [4], assuming a real countercurrent continuous movement of the solid catalyst phase. To increase the model reliability, special attention was paid to the determination and quantification of the reaction kinetics. As a representative VOC model system, the total oxidation of ethylene and propylene on a CrO_x/γ-Al_2O_3 catalyst was studied experimentally and theoretically. The oxidation reactions of the hydrocarbons were described successfully via an *Eley/Rideal* mechanism. The adsorption isotherm parameters were estimated independently based on additionally measured adsorption equilibria. In this way, the significance of the kinetic parameters in the rate model could be increased and a good agreement of the model with a large set of experimental data was achieved [5].

3. Results and discussion

For experimental investigation of the SMBR concept a pilot plant was designed and constructed. This test facility consisted of two adiabatic segments (L_{seg} = 0.5 m) equipped with several thermocouples placed in each reactor and several valves. In this plant, stable ignited operation could be experimentally maintained for over 120 hours. This allowed studying in detail the dynamics of the temperature fronts (see Fig. 1c). Based on the observed plant behavior a simplified reactor model as well as the model for the reaction kinetic could be evaluated and improved.

4. Conclusions

Trapping self-sustained exothermal reaction fronts inside the SMBR an energy efficient autothermal operation could be obtained, in which the feed mixture could be introduced at ambient temperature. The desired operation was achieved by shifting periodically the feed position in the direction of the flow when the reaction front leaves a currently active reactor segment. In this way, extinction could be avoided and a continuous operation mode was achieved. The Simulated Moving Bed Reactor is seen as an attractive energy efficient concept capable to perform efficiently heterogeneously catalyzed total oxidation reactions [6]. Future investigations are recommended to apply the concept also for other types of reactions, e.g. hydrogenations.

References

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Keywords
Simulated Moving Bed Reactor; Reactor Modeling, Experimental Investigation, Reaction Network Analysis, Kinetics