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Modelling of oxidative dehydrogenation of ethane to ethylene on NiSnO based catalysts in an industrial-scale packed bed catalytic reactor

Aim

The objective of the project is to study the catalytic behaviour of a NiSnO based catalyst for the oxidative dehydrogenation of ethane (ODH-C2) in a wall-cooled industrial-scale packed-bed reactor with a tube to particle diameter ratio below 5, making use of three mechanistic kinetic models: LHHW, ER and MvK and simulate the design on the process in the commercial software ASPEN TECH.

Justification

Ethylene is globally the most produced olefin and is an important raw material in the modern chemical industry. It is currently mainly obtained by steam cracking of different hydrocarbon streams and to a lesser extent also by fluid catalytic cracking (FCC). However, these processes present several disadvantages such as thermodynamic limitations, rapid coking, an ethylene selectivity below 60%, a costly product separation, and/or high energy consumption. Hence, the catalytic oxidative dehydrogenation (ODH) of ethane represents an attractive alternative technology for ethylene production. ODH has several advantages, first, it is an exothermic reaction that can already be carried out at relatively low temperatures (typically below 450 °C) using a suitable catalyst, second, the large-scale exploitation of shale gas has greatly increased the availability of ethane raw material. Finally, catalyst deactivation from coke formation is suppressed due to the presence of oxygen and lower operating temperatures.

There are several catalysts that are promising for ODH-C2, among others NiSnO based ones. This material has proven to be active already at low reaction temperature (<500 °C) and exhibit ethylene selectivities(> 80%). From this end, envisaging a possible future application of this material in ODH-C2 at the commercial scale requires, as a first step, a conceptual design of the catalytic reactor technology. The wall-cooled catalytic reactor with low tube-to-particle diameter ratio ($d_t/d_p < 5$) has showed to be suitable option, as shown by its success for other exothermic partial oxidation systems. The main advantage of this configuration is the fast removal of the generated heat, such that the ethylene yield can be maximized and severe catalyst deactivation is avoided. To carry out the study, several kinetic models than have been developed in the work group are available, and to test the performance of the industrial reactor by a set of simulations, a code developed in the Fortran interface is ready to use.

Program

- Literature survey on industrial packed bed reactors studies applied to highly exothermic reactions.
- Proposal of the simulation experimental design to identify the simulation of the main variables that affect the process.
- Carry out an a parametric sensitivity study, comparing the performance of the three kinetic models at industrial reactor lever scale.

Using the results obtained of the parametric sensitivity study to propose the design of the optimized process in ASPEN TECH