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Safety analysis of a heterogeneous catalytic tubular reactor for complex reactions

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Abstract

Probably chemical reactors represent the most hazardous units of the chemical industry. Safety analysis of a chemical reactor requires basic knowledge of all particular reactor processes.

The main goal of this work is the safety analysis of a heterogeneous catalytic reactor. Parametric sensitivity analysis, a part of safety analysis, has been done to reveal hazardous or noneconomic at range of the inlet parameters, like temperature and composition of the inlet stream, cooling media temperature or mass flow, initial temperature of the bed, etc. Results of the parametric sensitivity simulations can identify and describe the sensitivity of the reactor behavior to the variation of the chosen inlet parameters. These pieces of information can be useful to find safety and economical optimal design of the reactor.

This paper discusses partial oxidation of ethylene to ethylene oxide in a heterogeneous catalytic reactor which was chosen as the model system. A heterogeneous model with axial dispersion was chosen as the mathematical model of this reactor.

All simulations detect maximal reactor sensitivity or changes in performance parameters (oxygen conversion, ethylene selectivity to ethylene oxide or hot spots in the reactor) to any variation of the cooling media parameters (temperature, vaporating energy and flow rate). With such variations (e.g. linear increase of the cooling media temperature) not only the quality of the product is decreased (decrease of the ethylene selectivity to ethylene oxide) but potential dangerous situations can also be generated (increase of the oxygen conversion leading to high increase of the hot spot temperature).

Keywords:

tubular reactor, dynamic simulation, parametric sensitivity, complex reactions

1. Introduction

Exothermic reactions cause many problems during reactor operation. High production of the heat requires a very good cooling system of the reactor. Every change of the system parameters can cause large responses in the reactor behavior (increasing bed temperature, decreasing selectivity, starting of the undesired reaction, etc.). The question is which responses have been caused by changes of any system parameter (cooling, feed parameters). Answers could be given by safety and economic analyses of the system, e.g. reactor.

2. Problem Statement

Mathematical modeling could be useful for simulations of numerous devices, especially reactors. These simulations are helpful to find and to prevent most of the potential critical or dangerous situations of the chemical processes (mainly irreversible high - exothermic processes).

A fixed bed reactor with strongly exothermic reactions has been chosen as model system. Parametric sensitivity simulations give basic information about reactor behavior at changes of one or more system parameters. This information can be useful for more extensive safety analyses.

3. Paper approach

3.1. Methodology

A heterogeneous catalytic tubular reactor can be described by various mathematical models. In this paper a heterogeneous model with axial dispersion has been chosen. This model is one – dimensional and combines mass and energy balances with the transport mechanism model between fluid and solid phases, e.g. film theory [1, 2].

Absolute sensitivity is defined as a response of the system (change of reactor behaviour) to a random parameter (e.g. inlet temperature) which initiates some change in the system (e.g. key component conversion) [4].

3.2. Case study

As the model reaction system partial oxidation of ethylene to ethylene oxide has been chosen. The reaction system is as follows [3]:

$$O_2 + 2C_2H_4 \rightarrow 2C_2H_4O \qquad (R1)$$

$$O_2 + \frac{1}{3}C_2H_4 \rightarrow \frac{2}{3}CO_2 + \frac{2}{3}H_2O \qquad (R2)$$

where the first reaction (R1) is desired. The second reaction (R2) is more exothermic than the first. Both reactions are of first order with respect to oxygen concentration [4].

3.3. Results & discussions

Prior to the start of any safety analysis, parametric sensitivity simulations should be performed. These will reveal noneconomical or hazardous situations. Parametric selectivity to cooling media temperatures has been chosen as represent results of this paper.

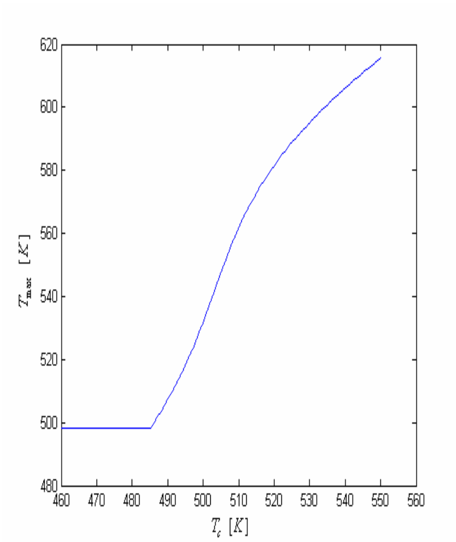

Figure 1: Maximal temperature in the reactor as a function of the cooling medium temperature

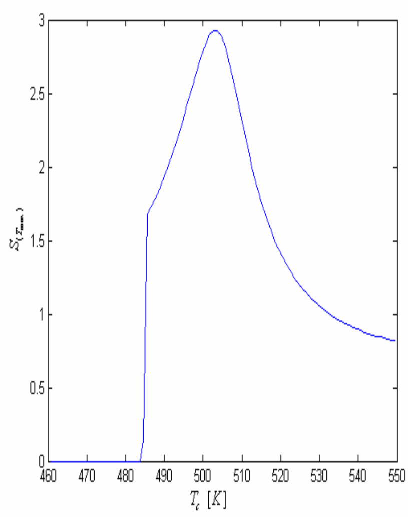

Figure 2: Objective parametric sensitivity to cooling medium temperature

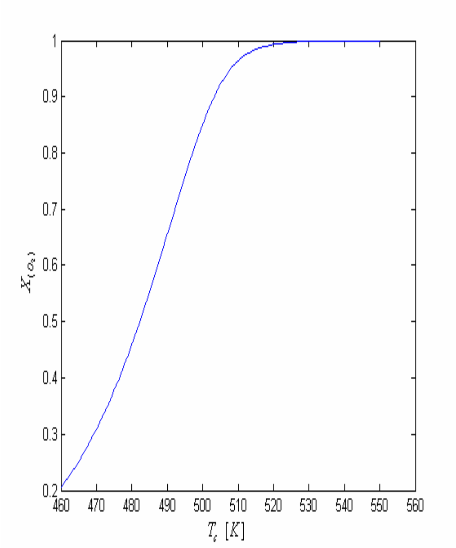

Figure 3: Oxygen conversion versus cooling medium temperature

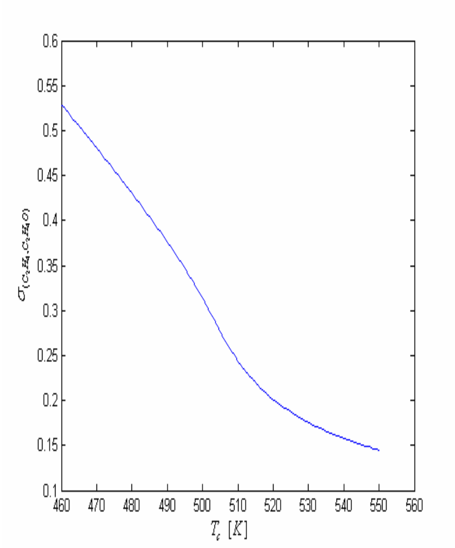

Figure 4: Selectivity to ethylene oxide as a function of the cooling medium temperature

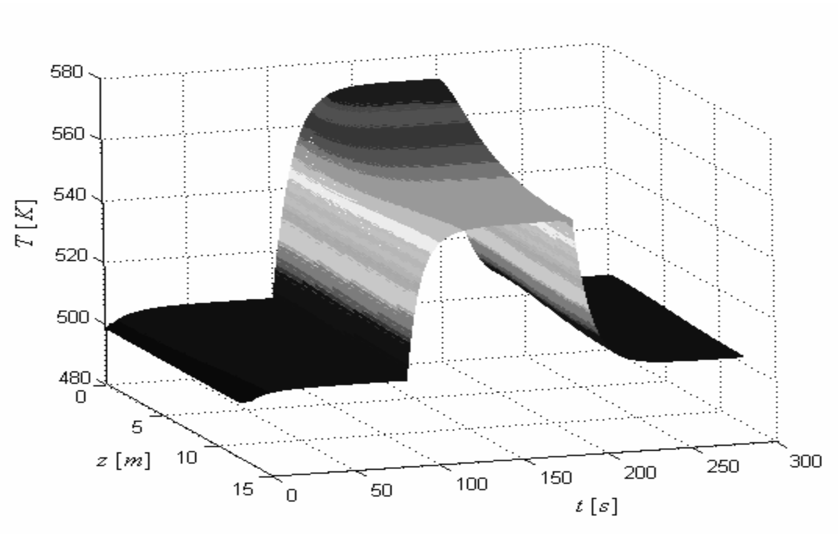

Figure 5: Temperature profile – start up of the reactor to steady state, step change of the cooling media temperature from 498 K to 548 K between 100 s and 200 sec of simulation time and consolidation to the previous steady state

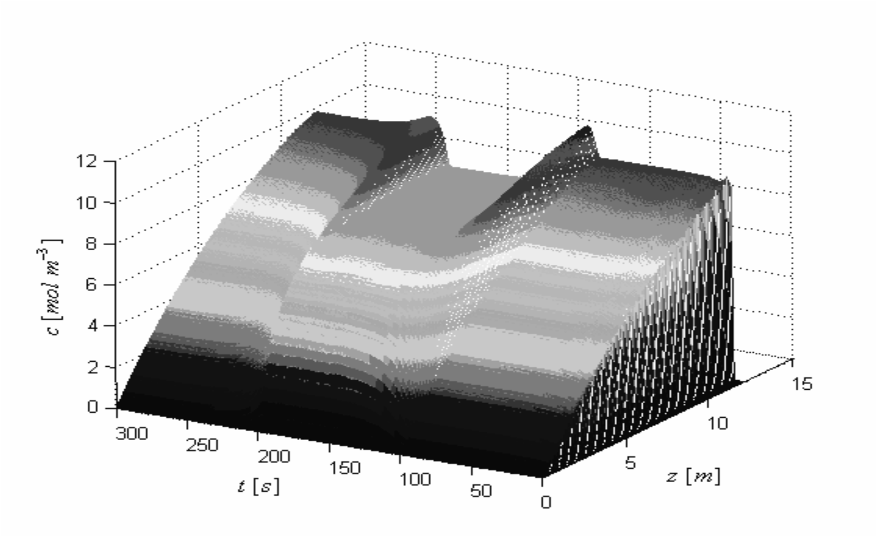

Figure 6: Ethylene oxide concentration profile – start up of the reactor to steady state, step change of the cooling medium temperature from 498 K to 548 K between 100 s and 200 sec of simulation time and consolidation to the previous steady state

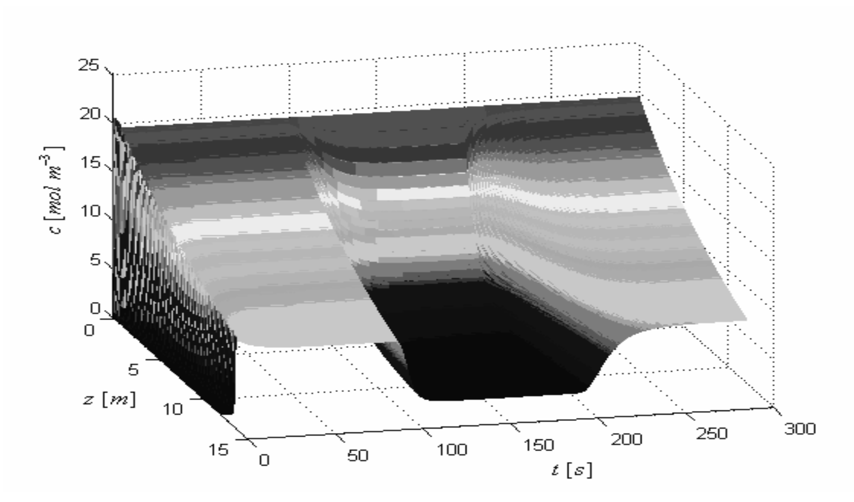

Figure 7: Oxygen concentration profile – start up of the reactor to steady state, step change of the cooling medium temperature from 498 K to 548 K between 100 s and 200 sec of simulation time and consolidation to the previous steady state

Figs. 1 – 4 represent reactor response to changes of the cooling media temperature. It can be seen that the sensitive range of the cooling media temperature is between 485 K and 520 K with maximal sensitive temperature of about 505 K. These figures illustrate that in the sensitive section of the reactor operations parameters, like maximal temperature (Fig. 1), selectivity to ethylene oxide (Fig. 4) or oxygen conversion (Fig. 3) is dramatically changed with respect to the changes out of this range. This phenomenon can be demonstrated by objective parametric sensitivity which is a function of the inlet parameter (Figs. 2).

Parametric sensitivity simulations refer sensitivity of the reactor between 485 K and 520 K of the cooling media temperature. Figs. 5 – 7 represent changes where the cooling medium temperature is jumped through this section from 498 K to 548 K and back. The time of the step change is between 100 sec to 200 sec of the simulation time.

4. Conclusions

The main aim of this work is the use of a mathematical model of a heterogeneous catalytic tubular reactor for safety analysis of such a reactor. Oxidation of ethylene to ethylene oxide was chosen as the model reaction system. Parametric sensitivity to changes of the cooling media temperature has been investigated. With such variations of the cooling (step change of the cooling medium temperature) not only the quality of the product is decreased, but potential dangerous situations can be generated. Rapid productions of ineligible products (increase of the oxygen conversion) cause rapid temperature increase (dangerous situations) and decrease of the ethylene oxide production (economical losses). This failure could cause increase of the pressure, reactor break - down, explosion, etc. These critical situations could be a goal of our further studies directed towards the oxidation of ethylene.

Acknowledgements

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References

1. Froment, G., F., Bischoff, K., B., Chemical Reactor Analysis and Design, John Wiley and Sons, New York, 1979
2. Vontruba, J., Hlaváček, V., Marek, M., Packed bed axial thermal conductivity, Chem. Eng. Sci., 1972, 27, 1845 - 1851
3. Westersterp, K. R., Ptasinski, K. J., Safe design of cooled tubular reactors for exothermic, multiple reactions, Chem. Eng. Sci., 1984, 39, 245 - 252
4. Slaback, D. D., Rigg, J. G., Time to runaway in a continuous stirred tank reactor, Ind. Eng. Chem. Res., 2004 ,43, 3723 - 3730