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Modeling and control of a novel heat exchange reactor, the Open Plate Reactor

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Abstract

A new chemical reactor, the Open Plate Reactor, is being developed by Alfa Laval AB. It combines good mixing with high heat transfer capacity into one operation. With the new concept, highly exothermic reactions can be produced using more concentrated reactants. A nonlinear model of the reactor is derived and a control system is developed. For temperature control a cooling system is designed and experimentally verified, which uses a mid-ranging control structure to increase the operating range of the hydraulic equipment. A Model Predictive Controller is proposed to maximize the conversion under hard input and state constraints. An extended Kalman filter is designed to estimate unmeasured concentrations and parameters. Simulations show that the designed control system gives high conversion and ensures that the temperature inside the reactor does not exceed a pre-defined safety limit.

Keywords: Heat exchange reactor; Process control; Mid-ranging control; Model predictive control; Extended Kalman filter; Process intensification

1. Introduction

The syntheses of fine chemicals or pharmaceuticals, widely carried out in batch or semi-batch reactors, are often strongly limited by constraints related to the dissipation of the heat generated by the reactions. A common solution is to dilute the chemicals to have lower concentrations, thus ensuring that the reaction rate and the subsequent heat release is lower than the heat transfer capacity of the reactor. After the reaction stage, the solvent is removed in a separation stage to provide a high-concentrated product of good quality. This separation process is both time and energy consuming, thus very expensive.

To reduce these problems, much research is performed within process intensification (PI), an engineering area where new methods and equipment are developed with the goal of allowing cleaner and more energy-efficient production using more compact design. The reduction in size also leads to increased safety with smaller amounts of hazardous chemicals being in use at each time. The field has been an active research area since the 1980s, see, for example, Ramshaw (1995), Green et al. (1999) and Stankiewicz and Moulin (2000). One example of PI innovation is the compact heat exchangers (HEX), which has been widely successful. However, attempts to use HEX as chemical reactors, to utilize their high heat transfer capacity, have had limited success due to the poor micro-mixing conditions. In the 1990s research on HEX reactors, to overcome these problems, started at the BHR Group Limited (Phillips et al., 1997) and also at Alfa Laval AB (Nilsson & Sveider, 2000).

A new concept of compact heat exchange reactors, the Open Plate Reactor (OPR) is being developed by Alfa Laval AB. It allows complex chemical reactions to be performed with a very accurate thermal control by combing high heat transfer capacity with improved micro-mixing conditions. Therefore, OPR appears particularly suited to process intensification, as it allows at the same time an increase of reactant concentration and a desired reduction of the solvent consumption. The reduced

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need of down-stream separation results in large savings in time and money. The improved heat transfer and mixing performance of the OPR, see Fig. 1, means that the OPR can replace larger conventional reactors, thus reducing plant size and investment costs. However, to take full advantage of the new reactor, a new process control system is also required. The main purpose of the feedback control, besides safety, is to facilitate the handling of the process, that is, adjust input variables to compensate for uncertainties in valves, pumps, heat transfer coefficients and reaction kinetics. With the large number of input variables it is non-trivial how to manually adjust them to optimize performance, while maintaining safe operation.

In this paper, the OPR is described from a control engineering perspective and a nonlinear first-principles model is derived. A control system is presented that is specifically designed to utilize the improvements of the new reactor design. The OPR is related to a plate HEX in that it has alternating reactor and cooling plates. The flow path is, however specifically designed to provide micro-mixing conditions superior to those in a HEX. Chemicals can be injected at multiple points along the reactor side so as to distribute the heat released from the reaction. In addition, numerous temperature sensors are mounted inside the reactor to monitor the process and to send measurement data to the process control system. For control purposes, the OPR can be approximated as an ideal tubular reactor.

There are a limited number of papers in the literature on the subject of control of continuous tubular reactors, but there is a wide range of different methods used for the control design. In Luyben (2001), the focus is on plant-wide control using a conventional control scheme. To control the maximum temperature inside the reactor, several internal sensors are used and their data are sent to a selector, which singles out the maximum temperature for feedback to a PI-controller. The main advantage is the simplicity of the feedback controller, however, it is not always trivial to find a suitable reference temperature for

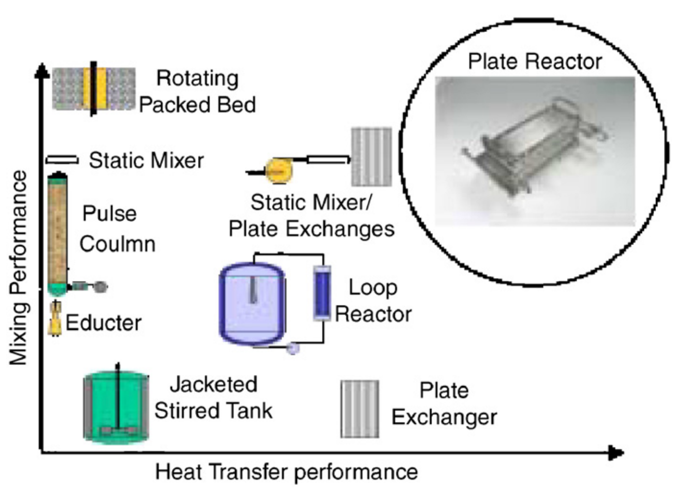

Fig. 1. Heat transfer performance and mixing performance for the OPR and other kinds of chemical reactors. Courtesy of Alfa Laval AB.

the reactor that gives optimal conversion. The effect of design and kinetic parameters on the controllability is also studied.

In Karafyllis and Daoutidis (2002) a nonlinear control law based on feedback linearization for a distributed parameter system is derived. The aim is to have the maximum temperature inside the reactor follow a desired reference temperature. The manipulating variable is the cooling temperature. The result is verified for both model and measurement errors. Also here, the choice of reference temperature is not discussed.

In Smets et al. (2002) optimal control theory is used to derive open-loop analytical solutions for the cooling temperature to maximize the performance. The performance criterion is defined as a combination of minimizing the outlet concentrations of the reactants and the global heat loss. One of the interesting results is the nearly optimal solution where a bang-bang cooling temperature profile is used. One cooling temperature is used for the first part of the reactor and after some switching point, another cooling temperature is used. This fits very well into the OPR framework, where the flexible configuration allows several different cooling flows to be used. However, limitations on the maximum reactor temperature are not considered and the open-loop control solution is sensitive to model uncertainties and process disturbances. The work has also been extended to tubular reactors with various degrees of dispersion, see Logist et al. (2005a, 2005b).

In Hudon et al. (2005) adaptive extremum seeking control is applied to a non-isothermal tubular reactor with unknown kinetics with interesting results. The main contribution is to allow for optimal control even in the presence of uncertainties, when the actual optimal operating point is unknown. The paper assumes that there are a finite number of control actuators to implement the calculated optimal cooling profile.

In Shang et al. (2002) characteristics-based model predictive control (MPC) is used to control the outlet concentration in a plug-flow reactor by manipulating the cooling flow rate. The main focus is on the significant computational benefits with the characteristics-based MPC compared to finite difference-based MPC. However, since an endothermic reaction is studied, the issue of hot spots and temperature constraints are not discussed in that paper. Other characteristics-based feedback control methods are described in Shang et al. (2005).

In the references above, all of the reactants are injected at the reactor inlet and consequently, the performance and safety of the reactor is controlled using only a single variable, in general the cooling temperature or flow rate. When there are multiple injections, the control strategies and methods need to be extended.

To accurately control the temperatures inside the OPR with these multiple injections, both the cooling temperature and the reactant injection flow rates are used as control variables. The multiple injections also change the dynamics and profiles of the reactor, compared to the examples