CHALLENGES IN START-UP CONTROL OF A HEAT EXCHANGE REACTOR WITH EXOTHERMIC REACTIONS; A HYBRID APPROACH

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Abstract: In this paper, the control of a continuous heat exchange reactor is investigated from a hybrid perspective with focus on the start-up phase and the transition to the optimal operating point. The temperature sensitive exothermic reaction leads to the possibility of multiple steady states and in combination with safety constraints forms an interesting challenge for a safe and efficient start-up. A series of MPC controllers are developed with a switching logic that transfers the process from initial rest to continuous optimal operation mode. The control procedure is verified in simulations with a full nonlinear model of the Open Plate Reactor, an improved heat exchange reactor being developed by Alfa Laval AB. The case study can be seen as a benchmark problem for start-up control of exothermic reactions.

Keywords: reactor start-up, hybrid control, heat exchange reactor, process control, model predictive control, exothermic reaction

1. INTRODUCTION

For industrial production of temperature sensitive exothermic reactions, safe and efficient start-up control is important.

Normally the reactor operates in a continuous mode around an optimal operating point. However, there are several different control modes associated with the production. In this paper, we will focus on the start-up mode, the continuous operation mode and the transition in between. We will show that it may be necessary to switch between several controllers with different optimization criteria to allow a safe and efficient start-up and thereafter optimal production.

The chemical reactor and the exothermic reaction form a highly nonlinear process and for some operating conditions also an unstable process. It is therefore essential that the reactor is started in a safe and accurate fashion. As shown later in Section 4, there can possibly be multiple steady states for a given process input, that is, applying the same process input may lead to different steady states depending on the current state of the process. The start-up phase is therefore non-trivial and much effort has to be used to ensure a safe operation.

In this paper, a hybrid control approach is used, where different controllers are used to transfer the process from initial conditions to a target region at the optimal steady state operating point.

The reactor studied in this paper is the Open Plate Reactor (OPR), currently being developed by Alfa Laval AB. It is a continuous heat exchange reactor, where the key concept is to combine efficient micro-mixing with improved heat transfer into one operation and it is further described in Section 2. The modeling and control of the OPR in the continuous operation mode is discussed in (Haugwitz and Hagander, 2006).

Many processes studied from a hybrid control point of view has a mixture of both continuous and discrete inputs, see e.g. (Stursberg, 2004), whereas the OPR only has continuous physical inputs. Instead, hybrid control may be required due to the multiple steady states of the OPR with both stable and unstable modes and the distributed actuation of the multiple inlet ports. This is further described in Sections 4 and 5.

2. THE OPEN PLATE REACTOR

The OPR consists of a number of reactor plates, in which the reactants mix and react. On each side of a reactor plate there is a cooling plate, through which cold water is circulated. In this paper a simple first order exothermic reaction is considered, see Eq. 1.

$$A + B \rightarrow C + D + \text{heat} \tag{1}$$

In Figure 1, a schematic figure of the first rows of a reactor plate is shown. The reactant A flows into the reactor from the upper left inlet. Between the inlet and the outlet, the reactants are forced by inserts to flow in horizontal channels in alternating directions. The inserts are specifically designed to enhance the mixing and at the same time the heat transfer capacity. The concept relies on an open and flexible reactor configuration. The type of inserts and the number of rows in the reactor plate, which determines the residence time, can be adjusted, based on the type and rate of the chosen reaction.

The reactant B can be added through multiple inlet ports, typically in the beginning and in the middle of the reactor. Temperature sensors can be mounted arbitrarily inside the reactor, specifically after each inlet port. To acquire accurate measurements of the temperature profile along the flow direction of the reactor, as many as 10 temperature sensors can be used. There can also be other sensors, such as pressure or conductivity sensors. The signals from the internal sensors are then used in the control system for emergency supervision and process control.

2.1 *Modelling*

A model of the OPR can be derived from first principles, with partial differential equations (PDE) for heat transfer, reaction kinetics, mass, energy and chemical balances, see for example (Thomas, 1999) or (Fogler, 1992).

The multiple consecutive horizontal channels inside the OPR in Figure 1, can be approximated as a continuous tubular reactor with axial dispersion with multiple inlet ports of reactant B along the reactor.

To simplify analysis of the PDE, which is an infinite dimensional system, the spatial derivative is approximated, using a first order backward difference method, as a finite system of ordinary differential equations (ODE). The model is discretized using n elements of equal size, where n can be a design parameter and may

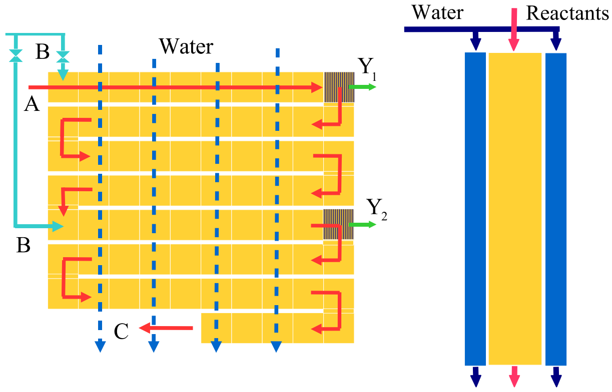

Fig. 1 Left: A schematic of a few rows of a reactor plate. Reactant A enters at top left and reactant B is added through several inlet ports along the reactor. Y_1 and Y_2 are internal temperature sensors used for process control and supervision. The cooling water flows from top to bottom in separate cooling plates. Right: The plate reactor seen from the side, with the reactor part in the middle and cooling plates on each side.

then be chosen such that the numerical dispersion approximates the actual dispersion of the reactor. The nonlinear model of the OPR is described in more detail in (Haugwitz and Hagander, 2006).

3. PROCESS OPERATION

There are four main control signals of the OPR; the feed flow rates of reactant B added at the two inlet ports, u_{B1} and u_{B2}, the inlet temperature of the cooling water T_{cool} and finally the inlet temperature T_{feed} of the reactant A, which constitutes the main part of the total reactor flow.

Of these four control variables, the two flow rates, u_{B1} and u_{B2}, are the most important, since they have the largest control gain from control signal to reactor temperature and they have the fastest actuator dynamics. Therefore, from a safety point of view, it is desirable to include the feed flow rates as control variables. However, changes in the flow rates may lead to stoichiometric imbalance so they should be used very carefully. T_{feed} and T_{cool} have lower control gains and slower actuator dynamics compared to the flow dynamics of u_{B1} and u_{B2}, but do not effect the chemical balance.

In some cases the total feed flow rate of reactant B is fixed to guarantee stoichiometric relations with reactant A, which flow is fixed. Then the control variable "feed flow distribution" u_B is used, that is, how large fraction of the total amount of reactant B that is fed through the first inlet port. The remainder $1 - u_B$ is then fed through the second inlet port.

4. START-UP DYNAMICS

As described in Section 2.1, the reactor is a distributed parameter system and is normally described with non-linear partial differential equations (PDE). Analysis of these infinite dimensional systems is quite difficult. Some results can e.g. be found in (Laabissi *et al.*, 2002) and references therein.

From (Laabissi *et al.*, 2002), it is known that there may be multiple steady states for a tubular reactor with axial dispersion. Similar effects may also be seen when there is significant heat storage and heat conduction in the axial direction inside the reactor. More references can be found in e.g. (Gray and Scott, 1990). The spatial discretization of the PDE into a system of ODEs used in Section 2.1 can also be viewed as the well known “tanks-in-series”-approximation, see e.g. (Fogler, 1992). To visualize the start-up dynamics, a simplified analysis is made based on this approximation. The numerical values used in this paper for the hypothetical reaction are found in Table 1.

In Figure 2, the process is simulated in open loop, for two different cases. The upper plot shows the reactor temperature around the first inlet port. The middle point shows the feed temperature of the reactant A and the lower plot shows the conversion of the reaction at the reactor outlet. Reactant B is added at time $t = 0$ through only one inlet port at the beginning of the reactor. The input conditions are identical for the two simulation cases, except for the feed temperature of reactant A. In the first case (dashed), the feed temperature remains constant at $T_{feed} = 20°$C. Almost no reaction occurs and the conversion is only 14 %. In the second case (solid) the reactant A is pre-heated during 30 seconds, but this is enough to temporarily increase the reaction rate. The exothermic reaction then releases heat itself, so when the pre-heating stops the reaction continues.

Another interesting part of Figure 2 is the sudden temperature increase around the inlet port at time t = 46 s as the pre-heating increases the reaction rate. The temperature increases 100°C within 1 second, which reveals the potential dangers during start-up. In fact, the heat release is so large that the safety limit at 150°, beneath which it is safe to operate, is violated quite rapidly. Without pre-heating, the conversion stays around 14 %, whereas with pre-heating it increases very quickly to almost 100% . It is then clear that with pre-heating the process is permanently moved from one stable equilibrium point to another, even though the input signals return to the same values. “Ignition” is said to have occurred when the process moves from an equilibrium at lower temperature to an equilibrium at a higher temperature. Note that there is a flow delay from the inlet port at the reactor inlet to the reactor outlet, which explains the delay from temperature increase at the inlet to the increase of the conversion at the reactor outlet.

Figure 2 shows that pre-heating of the reactants may be necessary to start the reaction. However, it may be dangerous to start feeding B before the pre-heating gives favorable conditions for the reaction rate. Even with closed-loop feedback control using the feed temperature as manipulated variable, there may still be safety issues due to slow actuator dynamics and model uncertainties. Therefore not only feedback control, but also the sequence of the start-up actions is critical as will be explained in the next section.

Ignition and safety aspects require pre-heating of the

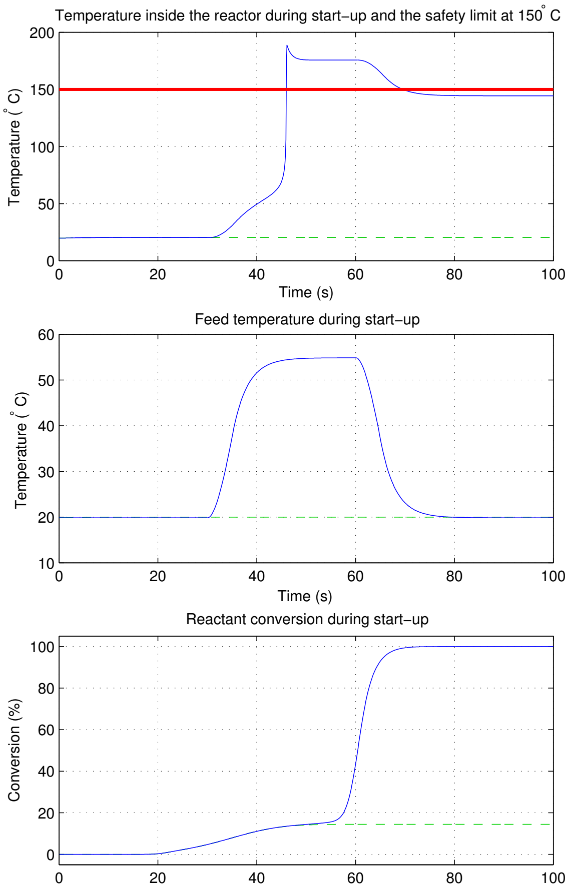

Fig. 2 The plot shows possible multiple steady states for the open loop system. If the steady state values of the inputs are applied from start, almost no reaction occurs inside the reactor (dashed). When a short time of pre-heating is done (solid), another steady state is reached.

Table 1 The data values used in simulations

Variable/Parameter	Value
Activation energy, E_a	77000 J/mol
Pre-exponential factor, k_0	2e7 m^3/(mol s)
Heat of reaction, ΔH	1.17e6 J/(mol m^3)
Feed inlet temperature, T_{feed}	20° C
Cooling temperature, T_{cool}	20°C

reactant, but on the other hand constant excessive pre-heating may not be desirable. When there are hard constraints in the reactor temperature, pre-heating may decrease the production capacity of the process. This means that we can feed less reactant B in the first inlet port if the temperature there is already high due to pre-heating. In addition, less pre-heating means less energy input being required.

To summarize, pre-heating of reactant A may be needed to start the reaction, the order of the start-up actions is important and the use of pre-heating should in steady state be as low as possible to allow high production rate of the reactor.

5. START-UP CONTROL OF THE OPR

The main rule is that no feeding of B should be made before the reactor temperature is such that the reaction starts immediately when adding B. If B is being fed and the reactor temperature is too low to allow sufficient reaction rate, there will be large quantities of unreacted chemicals inside the reactor. Then the risk of run-away reaction increases as seen in Figure 2, where feeding was started before the pre-heating was initiated. In this section one possible start-up control sequence will be presented.

During start-up the following control variables are available:

- u_{B1}, feed flow of B into the first inlet port
- u_{B2}, feed flow of B into the second inlet port
- T_{cool}, inlet temperature of the cooling water
- T_{feed}, inlet temperature of reactant A

The feed flows are defined as ratios of the total nominal flow of reactant B, that is, ranges from 0 to 1. In continuous operation, this flow is fixed to keep stoichiometric relations with reactant A, which has a fixed flow. However, during start-up this constraint is relaxed to improve safety and flexibility.

The following variables are to be controlled according to given reference values:

- T_1, the temperature in the reactor around the first inlet port
- T_2, the temperature in the reactor around the second inlet port

Since there are four control variables available to control only two temperatures, our control strategy uses two additional reference signals $u_{B1,ref}$ and $u_{B2,ref}$ for the two feed flow variables u_{B1} and u_{B2}. This penalizes deviations in these control signals from desired values during start-up. However, the controller can still use them to avoid violating constraints.

The start-up can be divided into the following steps, which are also graphically sketched in Figure 3:

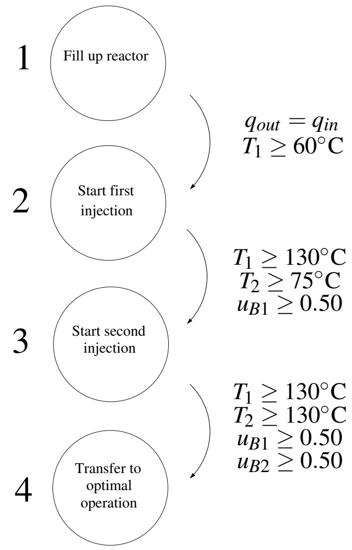

Fig. 3 State machine to illustrate the different steps during start-up and the guards corresponding to each transition. Note that the transitions are one-directional.

1. Fill the reactor with reactant A, which is pre-heated to 60°C. Wait until the outflow q_{out} equals the inflow q_{in}.

2. Start feeding reactant B in the first inlet port. The following reference values are used: $T_{1,ref} = 135°C$ and $u_{B1,ref}$ increases along a ramp from 0 to 0.5, which corresponds to 50% of the reactant B being added there. These references aim at obtaining a safe and reliable ignition of the reaction. The reference $T_{2,ref} = 80°C$ aims at giving good temperature conditions for the second inlet port, similar to the pre-heating before the first inlet port. And finally we are not allowed to feed anything into the second point until there has been a safe ignition at the first inlet port and there are favorable temperature conditions for the second inlet port, therefore $u_{B2,ref} = 0$.

3. Start feeding also in the second inlet port. As before $T_{1,ref} = 135°C$ and $u_{B1,ref} = 0.5$. $T_{2,ref}$ is set to 135°C and $u_{B2,ref}$ increases along a ramp from 0 to 0.5.

4. When the reactor temperatures have converged and feed flows reached their recommended values, the transition phase to the continuous operation mode begins. The controlled variables are now outlet concentrations of A and B, which should be controlled to zero. To fulfill stoichiometric relations, the feed flows of B are no longer controlled individually, but instead the distribution, u_B, between them is used, where $u_{B1} = u_B$ and $u_{B2} = 1 - u_B$. In addition, a reference value for the feed temperature $T_{feed,ref}$, is used to emphasize a low amount of pre-heating.

Whenever the guard conditions in Figure 3 have been fulfilled, a switch is initiated to the next step. During the entire start-up procedure, there is a critical safety constraint $T_{max} = 150°C$, so that all reactor temperatures should stay below that. This safety limit can be derived from by-product formation, cooling capacities or further exothermic side reactions.

5.1 *Implementing the start-up control*

It is possible to derive an open-loop start-up control procedure. However, it is non-trivial to find the best stationary operating point, while respecting the temperature constraints. In addition, it is difficult to find suitable open loop control trajectories to take the process from initial rest - through the ignition phase - to the optimal operating point. Model errors and disturbances may for some trajectories lead to hazardous operating conditions.

Therefore, the start-up procedure described above should be implemented with feedback control. The actual procedure is generic and is not restricted to any specific controllers. Alternatives can for example be PI-controllers with selectors or multivariable Model Predictive Control. Regardless of the chosen controller type, there will be a set of different controllers, one for each step of the start-up, see Figure 3.

In this paper, we have chosen to use MPC, due to its multivariable nature and its capacity to handle state constraints.

5.2 *Model Predictive Control*

A standard linear MPC controller was designed for each of the steps 2,3 and 4 in Figure 3, based on the notations of (Maciejowski, 2002) and algorithms from (Åkesson, 2003). The nonlinear process model was linearized at the switching point for each controller. Output feedback is implemented with an extended Kalman Filter (EKF), since only the temperatures are measurable. The concentrations inside the reactor and the feed concentrations are estimated by the EKF to improve robustness towards disturbances in the feed conditions. Due to lack of space, the details of the linear control design with MPC and EKF for the OPR can be found in (Haugwitz and Hagander, 2006).

6. SIMULATIONS

In Figures 4 and 5, the closed-loop start-up control procedure is simulated with the nonlinear process model. It is assumed that reactant A flows through the reactor and is being pre-heated to 60°C at time $t = 0$. This means that the switch between step 1 and 2, sketched in Figure 3, occurs at $t = 0$.

The MPC controller begins adding reactant B into the first inlet port at $t = 0$ s. As the feed flow increases the

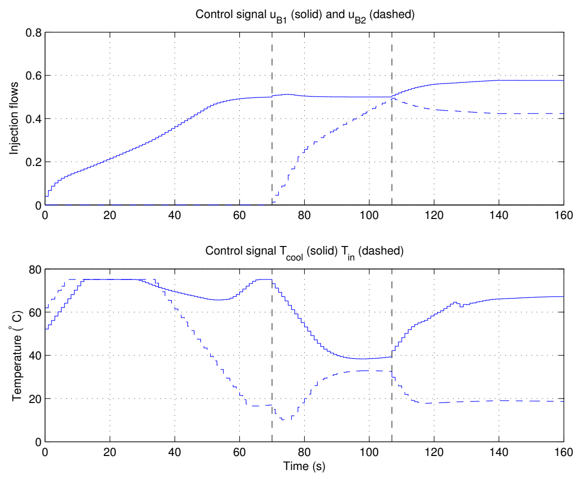

Fig. 4 Control signals during start-up procedure and transition to continuous operation mode. The vertical dashed lines indicate the switching times 70 s and 107 s.

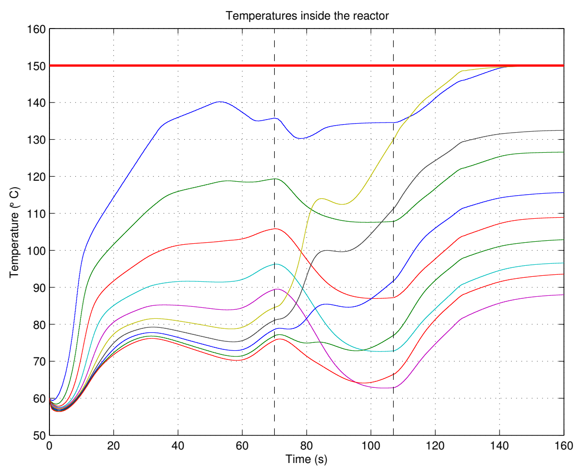

Fig. 5 Temperatures inside the reactor with the dashed line being the temperature at the first inlet port and the dash-dot line the temperature at the second inlet port. The vertical dashed lines indicate the switching times 70 s and 107 s.

controller has to decrease the pre-heating (with T_{feed}) to follow the temperature reference at $T = 135°C$. After 40 seconds, the temperature at the first inlet port has reached 135°C and the reaction has safely been ignited.

At $t = 70$ s the controller switches from step 2 to step 3 as the guard conditions from Figure 3 have been fulfilled. A MPC controller with different tuning parameters is used, but the main difference is that the feed flow rate at the second inlet port is now also included as a control variable. Again the aim is to track temperature references, now at the first and second inlet ports, and if possible follow control signal references for the two feed flows. As the second feed increases, the cooling is intensified and more pre-heating is again required.

At $t = 107$ s the guard conditions for transition between step 3 and 4 are fulfilled. The process has reached the pre-defined target region for the start-up procedure. Thus the controller switches mode from start-up mode to continuous operation mode. Another MPC controller is used, now with the aim of optimizing the conversion in the reactor. This is carried out by increasing the reactor temperature to the highest temperature allowed at which it is safe to operate. A secondary objective is to decrease the use of pre-heating. Therefore some reactant B is redistributed from the second to the first inlet port, which in turn decreases the need of cooling, thus saving energy.

At the end of the start-up, step 3, the conversion had reached 96.8% and after step 4, the transition to continuous operation mode, the controller has carefully adjusted the control signals, so that the conversion reaches 98.6 %. This is mainly due to operation closer to the reactor temperature limitations.

7. SUMMARY & CONCLUSIONS

The start-up control of a heat exchange reactor has been studied. The multiple steady states and multiple inlet ports along the reactor form a process with challenging dynamics. As seen in open loop simulations, the order of the start-up procedures is of great importance as well as the need for closed loop control.

The main rule is that the feed of reactant B should only start when there are favorable conditions for the reaction to ignite, especially in terms of reactor temperature. In this case, this means that the temperature of the reactants at each inlet port should be carefully controlled. To ensure safe start-up, a hybrid controller is presented, which step by step transfers the process from initial conditions to an operating point where the chemical conversion is maximized. In each step, a separate optimization criteria is used to ensure a safe transition using Model Predictive Control. MPC is also essential to handle safety constraints on the reactor temperatures. An extended Kalman Filter is designed to allow output feedback as concentration measurements are not generally available and to improve robustness for variations in feed conditions.

This case study can be seen as a benchmark problem for start-up control of exothermic reactions.

8. FUTURE WORK

To reduce the sensitivity to model errors from linearization, the start-up control procedure is currently being extended to nonlinear Model Predictive Control. It is then possible to take advantage of the available nonlinear process model. It will also be an interesting benchmark for NMPC, to see how it handle large transitions and the complicated ignition dynamics.

It would also be beneficial to use better and faster numerical algorithms to solve the optimization problems. This will allow faster sampling rate, which is desirable with the very fast ignition dynamics of the process.

Another approach in a different direction is to implement the same start-up control sequence using simpler controllers, such as Proportional-Integral controllers with selectors to allow constraint handling. This may be an interesting alternative as it is easier to implement in a industrial environment and may for several cases perform almost as good as the presented MPC solution.

Finally, it would be desirable to validate the process model with the real process with focus on parameters important for the start-up dynamics, such as thermal inertias, mass and heat dispersion coefficients and heat conduction in the axial direction.

9. ACKNOWLEDGMENTS

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