8th International IFAC Symposium on
Dynamics and Control of Process Systems
Preprints Vol.1, June 6-8, 2007, Cancún, Mexico

DYNAMIC OPTIMIZATION OF A PLATE REACTOR START-UP SUPPORTED BY MODELICA-BASED CODE GENERATION SOFTWARE

Staffan Haugwitz, Johan Åkesson and Per Hagander

Department of Automatic Control, Lund University
Box 118, SE-22100 Lund, Sweden
Email: {staffan.haugwitz, johan.akesson, per.hagander}@control.lth.se

Abstract: In this paper, start-up of a plate reactor is considered. Dynamic optimization is used to obtain start-up trajectories, and a feedback control structure for on-line control. The problem is challenging, since the process model is large and highly non-linear. In addition, the plant is subject to uncertainty. Special attention is given to the problem of formulating an optimal control problem based on physical insight. The robustness properties of the optimal solution are explored in simulation, by introducing parameter perturbations into the model. Automatic computer tools which greatly simplifies the task of formulating complex dynamic optimization problems are briefly discussed.

Keywords: dynamic optimization, process control, plate reactor, start-up, uncertainty, mid-ranging control, Modelica

1. INTRODUCTION

In this paper, start-up of the newly developed Alfa Laval Plate Reactor (Alfa Laval AB, 2006), is considered. This type of reactor is conceptually a combination of a tubular reactor and a plate heat exchanger. The key concept is to combine efficient micro-mixing with excellent heat transfer into one operation. Reactants can be injected at multiple points along the reactor length to enhance the reactor performance.

Start-up design has been an area of research for many years. In (Verwijs, et al., 1996), the start-up of an adiabatic tubular reactor system is studied. Open loop trajectories of the manipulated variables are calculated by optimization. The optimal trajectories of the manipulated variables are then implemented in open loop. In contrast to (Verwijs et al., 1996), the reactor in this paper is equipped with a cooling system and multiple injection points for reactants. In addition, feedback control is used to increase safety and robustness.

In (Haugwitz, et al., 2006), methods for modeling and control for stationary operating conditions of the plate reactor are presented. The present paper extends this work by proposing a method addressing the start-up problem for the plate reactor. Particular attention is given to the process of translating an informal specification into a formal optimal control formulation, supported by process insight.

We consider off-line optimization of start-up trajectories. There are mainly two reasons for this approach. Firstly, the size and complexity of the problem, in combination with fast dynamics complicates on-line solution of the optimal control problem. Secondly, a feedback system based on PID controllers has previously been designed and shown to give satisfactory performance for stationary operation. This control system can be used also during start-up. The optimal trajectories are then used as feedforward and reference signals. No changes of the control system are required.

The paper is organized as follows. The dynamic optimization method is described in Section 2. The plate reactor is briefly presented in Section 3. Section 4 outlines the specific problem formulation of the reactor start-up. Section 5 shows how the actual optimization problem is stated and the results of the optimization. The implementation of the closed loop control is presented in Section 6. The closed loop simulations are given in Section 7. The paper ends with conclusions in Section 8.

2. DYNAMIC OPTIMIZATION

We consider a direct simultaneous method, (Biegler, et al., 2002), for off-line optimization of start-up trajectories for the plate reactor. There are two main reasons for choosing a simultaneous method in this case. Firstly, the simultaneous methods have good numerical stability properties, which is important in this case, since the system dynamics is unstable in some operating conditions. Secondly, one of the most important elements of the optimization problem is a temperature path constraint, which is straight forward to enforce using a simultaneous method.

2.1 *Transcription Method*

A key element of a simultaneous method is the method used to discretize the differential equation. In this paper, we use orthogonal collocation over finite elements with Radau points and Lagrange polynomials, for its numerical stability properties. The purpose of the transcription procedure is to translate the infinite dimensional dynamic constraint into a finite dimensional constraint, which can be incorporated into the final algebraic non-linear program.

It is interesting to note that this collocation scheme can be shown to be equivalent to a fully implicit Runge-Kutta method. Accordingly, the strong stability properties, see e.g. (Petzold, 1986), of this class of methods are still valid.

2.2 *Tools*

Formulation of a dynamic optimization problem is an iterative process, which requires careful tuning of the cost function and the constraints. In addition, the properties of the numerical method used to solve the problem must be considered. The demanding task of *formulating* the problem is often complicated further by the details of how to *encode* the problem so that it fits the numerical algorithm. This encoding procedure is largely routine, but it is time consuming, error-prone and tends to distract the user from the key task of formulating the actual problem to be solved. Therefore, automatic computer software is important to bridge the gap between the requirements of the algorithms and the user's need of intuitive means to formulate the problem at hand. There is, however, a delicate balance between ease of use and restrictiveness when designing such software tools.

The plate reactor model is formulated in the modeling language Modelica, see (Modelica Association, 2000). Modelica is an object oriented language which enables the user to state mathematical equations declaratively. In addition, Modelica offers abstractions useful for structuring of large models, such as class inheritance, components and connection of components. There is a large number of free and commercial Modelica libraries covering application areas such as electronics, mechanics, thermo-dynamics, fluid mechanics and vehicles.

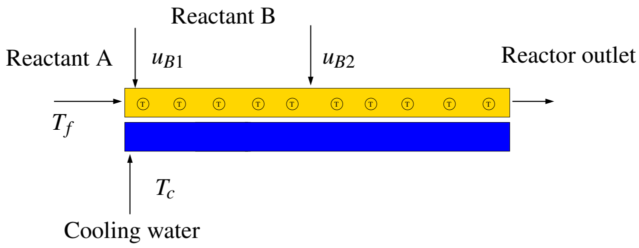

Fig. 1 The reactor shown as a schematic tubular reactor. There are four inflows to the process and there is one manipulated variable for each inflow; q_{B1}, q_{B2}, T_f and T_c. The circles with T represents internal temperature sensors.

In the optimization problem, the Modelica model represents the dynamic constraint. However, it is desirable to be able to express, formally, also the optimization quantities, such as cost and constraints. Therefore, a Modelica-based software tool offering support both for model descriptions given in Modelica *and* the optimization description is under development. This tool can be viewed as a front-end which can be used with different numerical algorithms.

The Modelica description of the process, and the complimentary description of the optimal control problem was automatically translated into AMPL, see (Fourer, et al., 2003), which is a language for mathematical programming. The translation was performed automatically using the software tools described above. The resulting NLP was solved using AMPL and IPOPT, which is an interior point optimization algorithm, (Wächter & Biegler, 2006).

3. THE PLATE REACTOR

In this section, the plate reactor is briefly described, for more details see (Haugwitz et al., 2006). The plate reactor consists of a number of reactor plates, where 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 second order exothermic reaction is considered.

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

In Figure 1, the plate reactor is schematically illustrated as a tubular reactor. The primary reactant A enters from the left. The secondary reactant B is injected at multiple points along the reactor. Between the inlet and the outlet, special inserts form flow channels of alternating directions that gives turbulent flows and good mixing of the reactants. The concept relies on a 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. With multiple injection points for reactants the production capacity can be increased and the reactor can be tailor-made for any complex reaction, e.g. multi-stage reactions. Temperature sensors can be arbitrarily mounted inside the reactor, specifically after each injection point.

3.1 *Inputs and outputs*

In this paper, we consider a reactor configuration with two injection points for reactant B and one single cooling flow, that is, the same water cools the entire reactor. The two injection points are located at the reactor inlet and mid section, respectively. Four control variables are used as manipulated variables in the optimization problem, see Figure 1. q_{B1} and q_{B2} are the two feed flow rates of reactant B added at the two injection points. In the sequel, we will use the scaled control variables $u_{B1} = q_{B1}/q_{feed,B}$ and $u_{B2} = q_{B2}/q_{feed,B}$, where $q_{feed,B}$ is a scaling factor. T_c is the inlet temperature of the cooling water and T_f is the inlet temperature of the reactant A, which constitutes the main part of the total reactor flow. Two temperature measurements located at the first and second injection point are used for feedback control.

Each control variable has a corresponding actuator system, so an input to the process is in fact a set-point to an actuator system. Therefore, in the sequel, $u_{B1,sp}, u_{B2,sp}, T_{f,sp}$ and $T_{c,sp}$ will be used, where $_{sp}$ stands for set-point.

3.2 *Modelling*

The plate reactor can be approximated as a continuous tubular reactor with multiple inlet ports of reactant B along the reactor. A model can be derived from first principles, using partial differential equations (PDE) for heat transfer, reaction kinetics, mass, energy and chemical balances, see for example (Froment & Bischoff, 1990). The reaction kinetics can be approximated using the Arrhenius law.

The PDE's are approximated with the Method-of-Lines using the finite volume method. The spatial derivatives are approximated with a first order backward difference method to a finite system of ordinary differential equations (ODE). Each PDE is approximated with $N = 30$ control volumes, which is a compromise between accuracy and computational complexity.

In each volume there are the following states; reactor temperature $T_{r,i}$, temperature of the cooling water $T_{c,i}$ and concentrations of substances A, B and C, that is, $c_{A,i}, c_{B,i}$ and $c_{C,i}$, where index $i = 1..N$ corresponds to the 30 control volumes. The injection of reactant B is approximated to be in control volume 1 and 16. In total, there are 154 continuous states, of which four are from the actuator models.

4. PROBLEM FORMULATION

The main problem is to transfer the states of the process from an initial point, where the reactor is cold and no reactant B is fed, to an optimal operating point with maximum reactant conversion. The main priority is safety, meaning that the temperature T_r throughout the reactor should at all times stay below a maximum limit, T_{max}. The secondary objective is to maximize the reactant conversions, γ_A and γ_B, defined as

$$\gamma_A = \frac{c_C}{c_C + c_A} \qquad \gamma_B = \frac{c_C}{c_C + c_B} \tag{2}$$

where c_A, c_B and c_C are the concentrations of A, B and C in the reactor outflow. With the reaction (1), this is equivalent to minimizing the amount of unreacted A and B in the reactor outflow.

The main challenges are the severe process non-linearities encountered during the start-up, limiting actuator dynamics and process uncertainty. There are many interesting problems associated with start-up of temperature sensitive exothermic reactions, (Haugwitz & Hagander, 2006). For example, there may be multiple equilibria for a given set of control signals. One equilibrium corresponds to the situation when no reaction occurs due to the low temperature. Another equilibrium occurs when almost all reactants have converted at high reactor temperature, which is the desired operating point. In between these points, there is also an unstable equilibrium point due to the fast temperature rise caused by the exothermic reaction.

5. THE OPTIMIZATION PROBLEM

5.1 *Specifications*

The mapping of the informal specifications given in Section 4 onto an optimal control formulation is non-trivial. In particular, there is a complicated inter-play between the feedforward trajectories and the closed loop system, which must be considered. The system model contains parameters which are uncertain, and the plant is also subject to disturbances. Therefore, enough control authority must be allocated to the feedback control system. This is done by enforcing more conservative constraints in the optimization procedure than is required by the physical plant. However, it is also desirable to reduce the start-up time in order to minimize off-spec products. Since this objective is in conflict with the objective of allocating enough authority to the feedback system, robustness and safety must be traded against performance. In this application, the safety requirements are most important, which is why these aspects are most emphasized in the paper. We will now discuss how the specifications can be formalized and expressed so that they can be incorporated in an optimal control problem.

State Transition The state of the reactor should be transferred from the cold stable equilibrium where no reaction takes place, to the hot stable equilibrium where the reactants A and B are converted to C. By minimizing the amount of reactants A and B at the outlet of the reactor, ignition of the reactor, and transfer of the state, can be achieved.

Accumulation of B For safety reasons, it is undesirable to have large amounts of substance B accumulated in the reactor during start-up. By studying linearization of the plant for different operating conditions, it is found that high concentrations of B at high temperatures yield unstable modes with fast dynamics. Since the authority of the feedback system is limited, these regions of operation should be avoided. Therefore, it is required that the concentration of B should not exceed a specified maximum level, in this application 200 mol/m^3 at the first injection point and 400 mol/m^3 at the second injection point. The constraints are chosen based on the steady-state values at optimal operation for the nominal model.

Reactor Temperature The reactor temperature, T_r, should not exceed the specified maximum temperature anywhere along the reactor length, in order to not damage the reactor. The maximum temperature should be chosen somewhat conservative, in order to allow for temperature fluctuations due to disturbances and parameter uncertainty. The maximum temperature allowed in the reactor is $T_{max} = 160°$C, while the corresponding temperature bound in the optimization problem was set to 155°C.

Rate Limitations of $T_{f,sp}$ and $T_{c,sp}$ Due to limitations in the feed heating system, the rate of change of the input $T_{f,sp}$ should be limited. Also, the limits for the rate of change should be chosen somewhat conservative in order for the feedback control system to have enough authority to compensate for modelling errors and disturbances. The physical rate limitations dictates that $-2 \leq \dot{T}_{f,sp} \leq 3$. In the optimization formulation, the bounds $-1.5 \leq \dot{T}_{f,sp} \leq 2$ were enforced. Similar limitations apply to the cooling system. While the physical limitations are given by $-2 \leq \dot{T}_{c,sp} \leq 1$, the bounds $-1.5 \leq \dot{T}_{c,sp} \leq 0.7$ were enforced in the optimization formulation.

Closed Loop Bandwidth Constraint Since the optimal control profiles will be used as feedforward signals, it is important to consider the robustness properties of the optimal solution. It is clear that a bang-bang solution, resulting e.g. from solving a minimum time problem, would not be robust, since the success of such a strategy is based on *timing*. If model uncertainty or disturbances are present, the timing of the bang-bang sequence might not match the state of the system, with deteriorated performance as a result. In this case, the optimal control profiles will be implemented by a feedback system. It is then convenient to formulate a specification for the control profiles in the frequency domain. Clearly, the feedback system cannot be expected to suppress disturbances or effects from model mismatch at frequencies higher than its bandwidth. Therefore, the frequency content of the control variables should be such that high frequencies are not injected into the system. This requirement can be achieved by introducing, into the optimization problem, high-pass filtered versions of the control variables, which are then used in the cost function. In this application, the bandwidth of the closed loop system is close to 0.5 rad/s. Accordingly, the bandwidth of the filter, ω_c^f was chosen to 0.5 rad/s. For comparison, the case of $\omega_c^f = 5$ rad/s was evaluated. The filter was implemented as a third order Butterworth high-pass filter.

5.2 *The Optimal Control Problem*

Given the specifications presented in the previous section, the optimization problem can now be written as

$$\begin{aligned}\min_u \int_0^{t_f} & \alpha_A c_{A,N}^2 + \alpha_B c_{B,N}^2 + \alpha_{B1} u_{B1,sp,f}^2 + \\ & \alpha_{B2} u_{B2,sp,f}^2 + \alpha_{T_1} \dot{T}_{f,sp} + \alpha_{T_2} \dot{T}_{c,sp} dt\end{aligned}$$

subject to

$$\begin{aligned} \dot{x} &= f(x,u) \\ T_{r,i} &\leq 155, \quad i = 1..N \quad c_{B,1} \leq 200, \quad c_{B,16} \leq 400 \\ -1.5 &\leq \dot{T}_{f,sp} \leq 0.7, \quad -1.5 \leq \dot{T}_{c,sp} \leq 2 \end{aligned} \tag{3}$$

where $u_{B1,sp,f}$ and $u_{B2,sp,f}$ are the filtered control variables corresponding to injection of substance B and α_i are weights. $c_{B,1}$ and $c_{B,16}$ are the concentrations at the first and the second injection point, respectively.

The problem was transcribed and solved as described in Section 2, using the automatic Modelica-based software. Scaling of variables and a good initial guess proved to significantly improve convergence of the algorithm.

5.3 *Optimization Results*

Two cases have been considered, $\omega_c^f = 0.5$ and $\omega_c^f = 5.0$ rad/s. The point is to show the trade-off between performance, here start-up time, and robustness. The optimal control profiles for both cases are shown in Figure 2. As can be seen, the first case when $\omega_c^f = 0.5$ gives a somewhat slower response, which is to be expected due to a more conservative frequency penalty on the control signals. In Figure 3, the state variables T_r and c_B are shown at the two injection points, where the maximum temperatures are achieved. Notice that the temperature constraints are active at the optimal steady-state operation point. In the case of $\omega_c^f = 5.0$, the reactor temperature approaches 155°C more quickly. This is expected since a higher value of ω_c^f results in more aggressive, but less robust control profiles, as there is less penalty on high frequency control signals. However, there is almost no difference in the settling time of the conversion, γ_A, so there

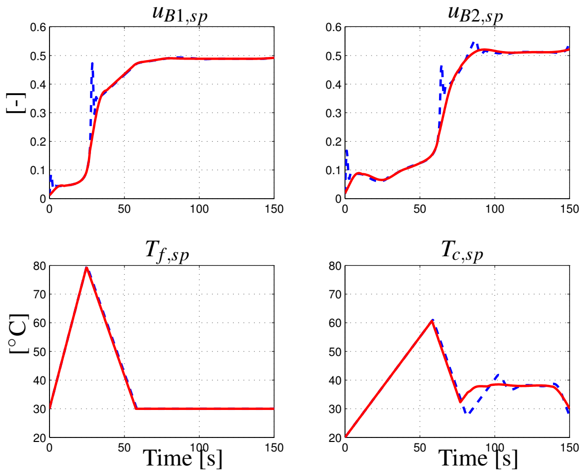

Fig. 2 Optimal control profiles. The dashed curves correspond to the case $\omega_c^f = 5.0$ rad/s and the solid curves corresponds to $\omega_c^f = 0.5$ rad/s.

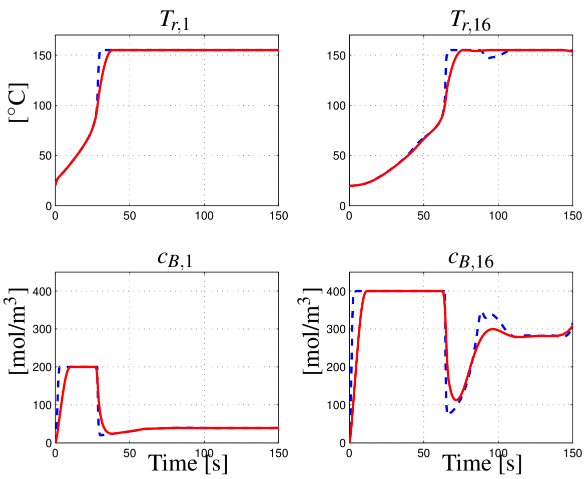

Fig. 3 Optimal profiles profiles for reactor temperature and concentration of substance B. The left plots correspond to the first injection point, whereas the right plots correspond to the second injection point. The dashed curves correspond to the case $\omega_c^f = 5.0$ whereas solid curves corresponds to $\omega_c^f = 0.5$.

seems to be almost no performance loss for increasing robustness in this case, compare also Figures 5 and 7.

The constraints on c_B, see Figure 3, ensure that there is only a limited ackumulation of unreacted chemicals in the reactor. This reduces the risk of uncontrolled ignition and increases the robustness.

6. CLOSED LOOP CONTROL

The dynamic optimization algorithm gives open loop trajectories for the four manipulated variables and the resulting reactor temperatures. Feedback control is necessary, however, due to process uncertainties and disturbances. For this purpose, the mid-ranging control structure, see e.g. (Åström & Hägglund, 2005), shown in Figure 4 is introduced.

The feed flow rates $u_{B1,sp}$ and $u_{B2,sp}$ have larger process gain and very fast impact on $T_{r,1}$ and $T_{r,4}$, but

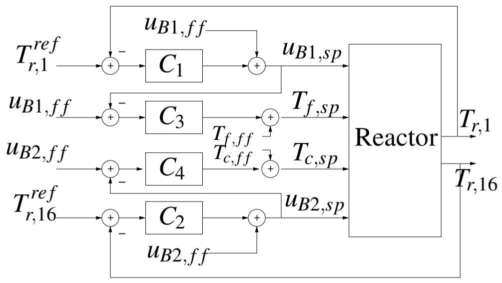

Fig. 4 Block diagram for the mid-ranging feedback control system.

they also affect the stoichiometric relation and should thus be used with care. Clearly, the variables $T_{f,sp}$ and $T_{c,sp}$ also affects the reactor temperature, but the given rate limits prevent achieving desirable bandwidth for the closed loop system using these inputs.

The idea of mid-ranging is to use control variables with fast impact, in this case, $u_{B1,sp}$ and $u_{B2,sp}$, to account for high frequency variations and variables with slow impact, in this case, $T_{f,sp}$ and $T_{c,sp}$, to account for low frequency variations. In this context, this means that deviations from the optimal trajectories can be effectively controlled during start-up. During stationary operation, the mid-ranging control structure ensures that the feed flow rates, u_{B1} and u_{B2}, return to the optimal values, while the feed and cooling temperatures account for modeling errors and constant disturbances. To reduce the interaction between the fast and the slow control variables, the slow control loops are designed to have a closed loop bandwidth that is an order of magnitude smaller.

7. SIMULATION RESULTS

To illustrate the need for robustness, the start-up simulation is performed with the heat transfer coefficient 10% lower, the heat of reaction 5% higher, the pre-exponential coefficient 5% lower and the activation energy 2% higher than in the nominal model. The reference trajectories used in the simulations correspond to the case when $\omega_c^f = 0.5$ rad/s.

Figure 5 shows the open loop and the closed loop response in presence of the model mismatch. The open loop response, without any feedback, leads to reactor temperatures at the two injection points around 163°C and 166°C, clearly above the maximum limit of 160°C. With feedback, the resulting temperature trajectories can hardly be distinguished from the references.

Figure 6 shows the control variables u_{B1}, u_{B2}, T_f and T_c and the feed forward trajectories from the optimization algorithm. When the reaction starts, the effect from the parameter errors forces the controller to adjust the feed flow rates to track the reactor temperature. Meanwhile, T_f and T_c are slowly manipulated to allow u_{B1} and u_{B2} to return to their optimal trajectories, thus

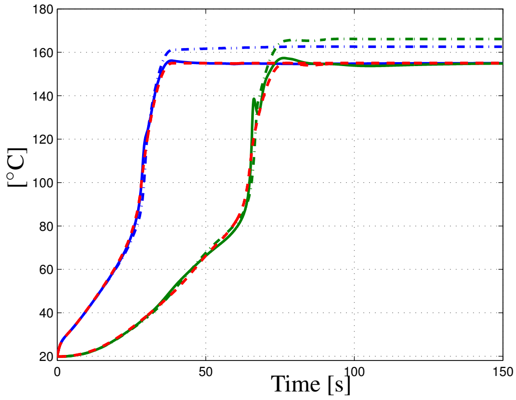

Fig. 5 Temperatures at the first and second injection point when the optimal inputs are applied to the perturbed system without feedback (dash-dot) and with feedback (solid). The solid lines can hardly be distinguished from the optimal references (dashed), with $\omega_c^f = 0.5$ rad/s.

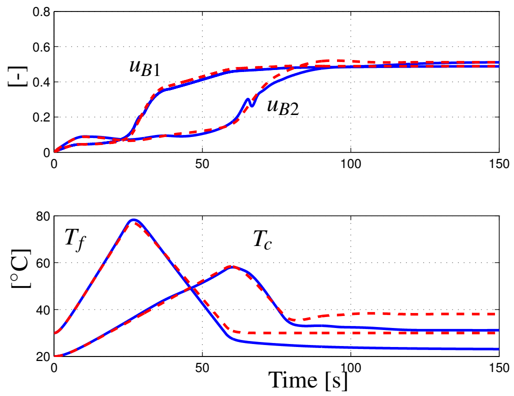

Fig. 6 The control variables during the closed loop simulation. The feed forward terms from the optimization are dashed and the actually applied control signals are solid.

ensuring optimal conversion. This illustrates nicely the characteristics of mid-ranging control, where u_{B1} and u_{B2} compensate for high frequency variations, while $T_{f,sp}$ and $T_{c,sp}$ account for the low frequency variations.

If reference trajectories corresponding to the case $\omega_c^f = 5.0$ rad/s are used, the feedback controller can not compensate fast enough for the effects of the model mismatch. With the parameter errors above, there will be an overshoot to 170° C, due to lack of robustness of the reference trajectories, see Figure 7.

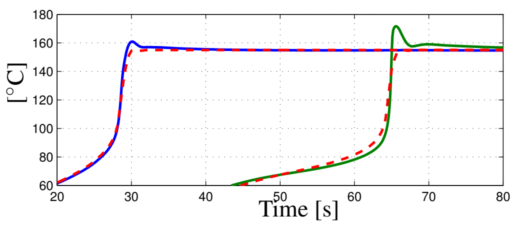

Fig. 7 The reactor temperatures when $\omega_c^f = 5.0$ rad/s.

8. CONCLUSIONS

In this paper, it has been shown how dynamic optimization can be used to generate trajectories for starting a plate reactor. The complex inter-play between the formulation of the optimization problem and the implementation of its solution in a closed loop setting has been discussed. The proposed solution has been evaluated, in simulation, under the assumption of uncertain parameter values, with satisfactory result.

The design procedure has been supported by automatic code generation tools, where the model description has been expressed in Modelica. The availability of automatic tools has enabled focus to be shifted from the details of *encoding* the problem towards *formulation* of the actual optimization problem. As a result, the iterative process of formulating a dynamic optimization problem is supported. A natural extension of this paper is to to further explore the robustness properties of the optimal profiles and evaluate the designed start-up trajectories with Monte Carlo analysis.

9. REFERENCES

Alfa Laval AB (2006). 'Alfa Laval Reactor Technology'. http://www.alfalaval.com.

K. J. Åström & T. Hägglund (2005). *Advanced PID Control*. ISA - The Instrumentation, Systems, and Automation Society, Research Triangle Park, NC 27709.

L. Biegler, et al. (2002). 'Advances in simultaneous strategies for dynamic optimization'. *Chemical Engineering Science* **57**:575–593.

R. Fourer, et al. (2003). *AMPL – A Modeling Language for Mathematical Programming*. Brooks/Cole — Thomson Learning.

G. Froment & K. Bischoff (1990). *Chemical reactor analysis and design*. Wiley.

S. Haugwitz & P. Hagander (2006). 'Challenges in Start-Up Control of a Heat Exchange Reactor with Exothermic Reactions; A Hybrid Approach'. In *Proceedings of the 2nd IFAC Conference on Analysis and Design of Hybrid Systems*, Alghero, Italy.

S. Haugwitz, et al. (2006). 'Modeling and Control of a Novel Heat Exchange Reactor, the Open Plate Reactor'. *Control Engineering Practice* In press, available online through DOI using doi:10.1016/j.conengprac.2006.02.019.

Modelica Association (2000). *Modelica - A Unified Object-Oriented Language for Physical System Modeling*. www.modelica.org.

L. Petzold (1986). 'Order Results for Implicit Runge-Kutta Methods Applied to Defferential/Algebraic Systems'. *SIAM Journal on Numerical Analysis* **23**(4):837–852.

J. Verwijs, et al. (1996). 'Startup Strategy Design and Safeguarding of Industrial Adiabatic Tubular Reactor systems'. *AIChE Journal* **42**:503–515.

A. Wächter & L. T. Biegler (2006). 'On the implementation of an interior-point filter line-search algorithm for large-scale nonlinear programming.'. *Mathematical Programming* **106**(1):25–58.