Modeling and simulation of a multi phase semi-batch reactor

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Abstract

The operation of an industrial semi-batch reactor, in which the bulk chemical EHEC, ethyl hydroxyethyl cellulose, is produced, is studied and simulated. In the reactor a strongly exothermic polymerization reaction takes place followed by a slightly exothermic reaction, and we want to minimize the duration of the operation of the process. Various operational as well as quality and safety related constraints have to be met during the batch. The complete process model, derived from measurements, first principles, and reasoning about effects on molecular level, is stated. The model includes heat and mass balances of the reactor, a pressure model, models of PID controllers, the jacket and the condenser. Technical limitations, for instance maximal and minimal jacket temperature changes due to limitations in the heat exchanger, have been modeled as constraints.

The equations have been implemented in SIMULINK, MATLAB and the model predicts the process variables rather well over time. During the first reaction, the model is not able to reproduce the jacket temperature to the desired accuracy, but the other variables have acceptable predictions. An optimization problem is formulated, wherein the total batch time is minimized under the constraints of the differential algebraic equation system and other constraints originating from the process, for instance limited pump capabilities.

As a first step in optimizing the operation of the process, a series of simulations has been performed in order to decrease the total batch time. It is concluded that a 10 % shorter batch time than today is possible if the quality is discarded, and a 5 % shorter batch time can be reached while using the existing requirements for the quality.

Keywords: Semi-batch reactor, simulation, optimization

1 Introduction

1.1 Optimization of batch reactors

In a batch process, the materials are loaded, the process is initiated, and after the reactions are completed, the products are removed. Hence, the conditions within the process are changing. The technology for making a given product is contained in the product recipe that is specific to that product [18]. The recipes are typically based on heuristics and experience. By the term semi-batch we means processes in which some parts are continuous but others are of batch type. For instance, in semi-batch operation a gas of limited solubility may be fed in gradually as it is used up.

Batch reactors are popular in practice because of their flexibility with respect to the duration of the chemical reaction and to the kinds and amounts of reactions that they can process. Generally batch processes are less safe, both for people and the environment, and the variations are smaller than in continuous processes [12]. In industry, batch and semi-batch reactors are often used in the production of fine chemicals, specialties, polymers and other high value products. Batch reactors are typically used when production volumes are low, when there are many processing steps, when isolation is required for reasons of sterility or safety, and when the materials involved are difficult to handle. The plants are often small and flexible, and the raw material and the products are expensive, but they can also be used in large volumes. They are primarily employed for relatively slow reactions of several hours duration, since the down time for filling, emptying and cleaning the equipment may be about one hour.

Chemical processes are modeled dynamically using differential algebraic equations (DAEs), consisting of differential equations that describe the dynamic behavior of the system, such as mass and energy balances, and algebraic equations that ensure physical and thermodynamic relations. Batch systems are difficult to study numerically due to the fact that steady state is never reached. In addition, chemical processes are typically nonlinear. In order to improve their performance and safety conditions, batch reactors generally require knowledge about the dynamic behavior, for instance through a mathematical description of the kinetics. The development and validation of detailed dynamic models are often quite expensive, why there is, in contrast to continuous processes which have been rigorously studied, a limited availability of detailed dynamic models. For bulk chemicals, the cost of developing models is rarely taken. Instead, the operators use experience to adjust the process periodically. Verwater-Lukszo [18] addresses this issue.

Starting as a technology in applications, mainly through operations research in the sense of optimizing complex systems and phenomena, optimization gradually became an area of academic interest. In the process systems engineering, on the contrary, it has evolved from an academic interest into a technology that has and continues to make a significant impact in industry. The increased competition in industry makes process optimization a natural choice for reducing production costs, improving product quality and reducing product variability. Often the objective in optimization of batch and semi-batch reactors is economic in nature, for instance reducing operational costs. Typically, operational decisions such as temperature and feed flow rates are determined from the optimization problem, and various operational constraints are considered. The practice of, and optimization challenges in, batch chemical industry is addressed by Bonvin et al. [4]. Overviews of the research on optimization of batch reactors until 1998 can be found in Rippin [14] and Bonvin [3]. Generally, the industry has a limited acceptance for optimization based techniques for the determination of operational profiles: to develop and validate detailed dynamic models is often considered too expensive to be motivated.

1.2 Optimal control problems

A general continuous optimal control problem, with the control variable u, and state variable x, is written as follows:

$$
\begin{aligned}
\text{minimize} \quad & f = \int_0^{t_f} L(x(t), u(t), t)dt + \phi(x(t_f)) && \text{(1a)} \\
\text{s.t.} \quad & h(\frac{dx}{dt}(t), x(t), u(t), t) = 0, && \text{(1b)} \\
& g(x(t), u(t), t) \leq 0, && \text{(1c)} \\
& x(t) \in X, u(t) \in U, && \text{(1d)} \\
& x(0) \in X_0, x(t_f) \in X_f, && \text{(1e)} \\
& t \in [0, t_f]. && \text{(1f)}
\end{aligned}
$$

Minimum-time problems, which is the type of optimization problem we have in this work, are optimal control problems in which it is required to go from some initial state to some terminal state in a minimum amount of time.

$$
\begin{aligned}
&minimize && t_f && \text{(2a)} \\
&s.t.\, for\; t \geq 0 && h(\dot{x}(t), x(t), u(t), t) = 0 && \text{(2b)} \\
& && g(x(t), u(t), t) \leq 0 && \text{(2c)} \\
& && x \in X, u(t) \in U && \text{(2d)} \\
& && x(0) \in X_0, x(t_f) \in X_f && \text{(2e)}
\end{aligned}
$$

Optimization problems can be classified in terms of continuous or discrete variables. For continuous problems an important distinction is whether the problem is differentiable or not. Another important distinction, for both types of problems, is whether the problem is convex or nonconvex, since the latter may give rise to multiple local minima.

1.3 Dynamic optimization methods

A continuous optimal control problem, Equation (1), can be solved either by Calculus of variations (indirect methods) or by applying some level of discretization that converts the problem into a discretized problem (direct methods) [2]. If the optimization will be performed in combination with an existing simulator, a direct sequential method is the first choice.

The variational approach, resulting in indirect methods, is based on the solution of the first order necessary conditions for optimality, that are obtained from Pontryagin's Maximum Principle [13], which results in a Two Point Boundary Value Problem (TPBVP). This TPBVP can be solved with different approaches, including single shooting, invariant embedding, multiple shooting, or some discretization method such as collocation on finite elements or finite differences [6].

In direct methods, the problem is parameterized by a finite number of parameters, transforming the continuous optimization problem to a discretized optimization problem. These methods use NLP solvers, and can be divided into two groups, sequential and simultaneous strategies. A general drawback is that the quality of the solution depends on the parametrization. In simultaneous methods all variables are discretized, and the dynamic equation is solved implicitly, simultaneously with the optimization problem. This results in large nonlinear optimization problems, which require specialized methods. The simultaneous methods couple the DAE to the optimization problem, and the DAE is solved only once at the optimal point. An advantage of these methods is that they are applicable to general problems. The methods are advantageous for problems with path constraints and also for problems where instabilities occur for a range of inputs, since they are able to suppress unstable nodes by enforcing the appropriate boundary condition. A disadvantage is the need to solve large nonlinear problems. A review of simultaneous methods can be found in [6]. Examples of methods that can be used to solve the NLP are Successive Quadratic Programming (SQP) [7], single shooting, multiple shooting [10] and direct shooting method (which is a bridge between direct and indirect methods), invariant embedding, global orthogonal collocation, orthogonal collocation on finite elements [5, 19], and moving finite elements [2].

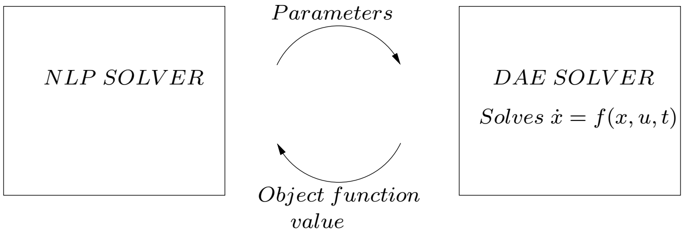


Figure 1: In sequential methods, each iteration the NLP solver sends values of the control parametrization to the DAE solver, which solves the equation $\dot{x} = f(x, u)$. This produces a value of the objective function which is used by the NLP solver to find the optimal parameters in the control parametrization.

In sequential methods, also called Control Vector Parametrization (CVP) [1], the control vector u is discretized (piecewise constant, piecewise linear or piecewise polynomial), and the dynamic equation $\dot{x} = f(x, u)$ is solved explicitly in each optimization step, with well-known integration, which means that also a non-optimal solution is feasible, Figure 1. Advantages of these methods are that they can handle rather large problems without large scale optimization techniques, and that a non-optimal solution is feasible. These methods run into problems, if the optimization algorithm requires gradient information, because standard DAE solvers are not usually written to provide parametric sensitivities of the solution, or, if provided, they might not be accurate enough for highly nonlinear models.

1.4 Objectives

In this study, a bulk chemical is produced in a semibatch reactor. We want to show that also small models can be used to gain knowledge when optimizing a semibatch process. In our model, two PID- regulators are included, in addition to mass and energy balances. Our semibatch process works reasonably well today. However, the set point temperature and set point pressure profiles are more or less based on experience, and measurements during batches show that with the existing equipment, these profiles are quite difficult to follow. Also, measurements on the resulting product implies that the prevailing settings gives a product with larger variations of the properties between batches than wanted. If the temperature can be better controlled the variation between batches can be decreased, with a more homogeneous product as a result. In this work, which is a first step in optimizing the operation of the process, we minimize the total batch time, without changing the slopes in the set point temperature profile or set point pressure profile and keeping the existing equipment.

We handle the dynamics of the cooling system by adding constraints on the dynamics and we assume that the control system is fast enough in order to implement the new trajectories. We do not have access to sensitivity information for the objective function and the constraint states with respect to the free optimization variables, as Abel et al. [1] do. Compared to Khuu et al. [9], in which the reactor content is preheated to the reactor temperature before EO is added, we include the heating in our study. Also we have limited access to reaction kinetics.

In this work we focus on a sequential method for optimization.

2 The model

2.1 Process description

In the reactor alkali cellulose is reacted with ethylene oxide (EO) and gaseous ethyl chloride (EC) under pressure and increased temperature, to produce EHEC, (Ethyl HydroxyEthyl Cellulose), a thickener in water-based systems. The reactions are described by:

$$\begin{aligned}
\mathrm{Cell-OH+OH^-} &\rightarrow \mathrm{Cell-O^-+H_2O} \\
\mathrm{Cell-O^-+nEO} &\rightarrow \mathrm{Cell-O-(EO)_n^-} \\
\mathrm{Cell-O-(EO)_n^-+EC} &\rightarrow \mathrm{Cell-O(EO)_n-Et+Cl^-} \\
\mathrm{Cell-O^-+EC} &\rightarrow \mathrm{Cell-O-Et+Cl^-}
\end{aligned}$$

The EO is added to the reactor as a liquid and vaporizes. In our process, the distribution of phases inside the reactor is not known. Possibly three phases are present, and it is also not known in which phase the reactions take place.

The temperature in the reactor is controlled by two separate systems; a condenser and a jacket, cf. Figure 2. The water in the jacket is circulated through a cold water inlet, through a heat exchanger to the reactor jacket, passing by an outlet where surplus water can be removed to keep pressure constant on the way back to the cold water inlet. The flow through the jacket system, F_j, is kept constant at a high level with a pump. In the heat exchanger steam is used as heating agent and the temperature of the cold, so called raw, water varies slightly during the year. The flow in the jacket is much higher than in the condenser. Two PID-regulators control the temperature of the jacket flow and the flow through the condenser, and the temperature and the pressure in the reactor is measured.

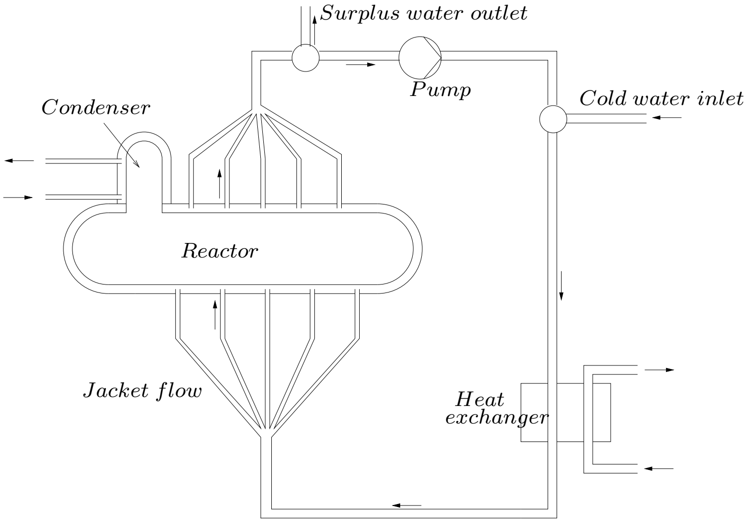


Figure 2: A process schematic, showing the jacketed reactor with the condenser to the left. The jacket system consists of the reactor jacket, outlet, pump, inlet and heat exchanger.

2.2 Model equations

The complete process model, derived from measurements, first principles, and reasoning about effects on molecular level, is stated below. All variables are scaled and uncertainties are not included in the model. The overall mass balance over the reactor, with units kg:

$$m_{tot}(t) = \sum_{\substack{All \\ Substances\ i}} m_i(0) + \int_0^t \dot{m}_{EO}(\tau)\, d\tau. \tag{3}$$

The overall heat balance, with units kJ/s, over the reactor, assuming $C_{P,tot}$ is constant:

$$\begin{aligned}\frac{\partial}{\partial t}(m_{tot}(t)C_{P,tot}T_r(t)) &= Q_{in}(t) - Q_{out}(t) + Q_r(t)\\ &= Q_{in}(t) - Q_j(t) - Q_c(t) + Q_r(t),\end{aligned} \tag{4}$$

where heat content in the EO-addition is:

$$\begin{aligned}Q_{in}(t) = \frac{\dot{m}_{EO}(t)}{M_{EO}}&[\Delta H^{EO}_{vap}(T_0)\\ &+ C^{gas}_{P,EO}(T_r)T_r(t) - C^{gas}_{P,EO}(T_0)T_0],\end{aligned}$$

with

$$\begin{aligned}\Delta H^{EO}_{vap}(T) &= A(1 - \frac{T}{B})^C,\\ C^{gas}_{P,EO}(T) &= a_0 + a_1 T + a_2 T^2 + a_3 T^3 + a_4 T^4.\end{aligned}$$

The heat transfer Q_j from material inside the reactor to the jacket water is (the units are kJ/s):

$$Q_j = k_j A_j (T_r(t) - \overline{T}_j(t)),$$

and to the condenser average temperature:

$$Q_c = U_c(t) A_c (T_r(t) - T_{c,in}(t)),$$

where

$$U_c(t) = \frac{1}{\frac{1}{k_c A_c} + \frac{1}{2F_c(t)\rho_w C_{P,w}}}.$$

The reaction heat Q_r is given by

$$Q_r(t) = \Delta H_{EO} r_{EO}(t) + \Delta H_{EC} r_{EC}(t),$$

with the reaction rates r_i:

$$\begin{aligned}\frac{\partial c_{\mathrm{EO}}}{\partial t} &= - r_{EO'} = -k_{EO}(T)c_{\mathrm{EO}},\\ \frac{\partial c_{\mathrm{EC}}}{\partial t} &= - r_{EC'} = -k_{EC}(T)c_{\mathrm{EC}}c_{\mathrm{RO^-}},\\ \frac{\partial c_{\mathrm{RO^-}}}{\partial t} &= - r_{RO^-{}'} = -k_{RO^-}(T)c_{\mathrm{EC}}c_{\mathrm{RO^-}}.\end{aligned}$$

Here the reaction constants k_i are given by Arrhenius equation $k_i(T(t)) = A_i exp(-\frac{E_i}{T(t)})$.

We include two PID-regulators, each described by the following equation, with all variables expressed in percents:

$$u = K\left(r - y + \frac{1}{T_I}\int (r-y)\, dt - T_D\frac{dy}{dt}\right). \tag{5}$$

In the condenser, $u = F_c/F_{c,Max}$, $y = P_r/P_{Max}$ and $r = P_{set}/P_{Max}$ and in the jacket $u = T_j/T_{Max}$, $y = T_r/T_{Max}$ and $r = T_{set}/T_{Max}$.

In order to fully describe the system we also need an expression for the reactor pressure:

$$\begin{aligned}P_r &= P_{EO} + P_{EC},\\ P_{EO} &= P^o_{EO}(T)(\alpha_1 n_{EO}(t) + \beta_1),\\ P_{EC} &= P^o_{EC}(T)(\alpha_2 n_{EC}(t) + \beta_2)(\gamma_1 \lambda_{EO}(t) + \delta_1),\end{aligned}$$

where $P_i^o(T_r)$, the vapor pressure for species i, and $\lambda_{EO}(t)$, describing the progress of the EO-reaction, are given on the form

$$\begin{aligned} P_i^o(T_r) &= 10^{(A+\frac{B}{T+C})}, \\ \lambda_{EO}(t) &= \frac{n_{EO,reacted}(t)}{n_{EO,reacted}^{max}}. \end{aligned}$$

The set point curves for temperature and pressure are shown in Figure 3, as well as the original EO-profile.

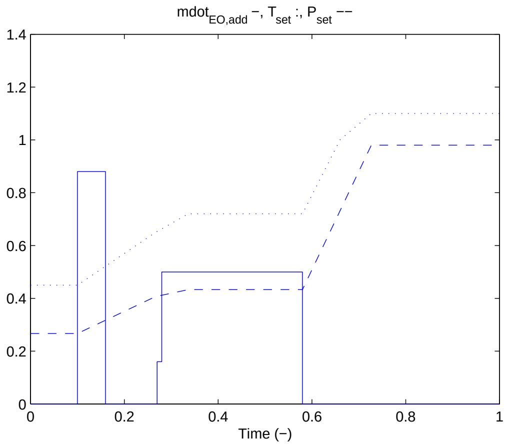


Figure 3: The figure shows the set point curves for temperature T_{set}, and pressure P_{set}, and the original EO-addition $\dot{n} = mdot_{EO,add}$.

This system is simulated in SIMULINK, with the result shown in Figures 4 and 5. As can be seen, all simulated curves but the jacket temperature follow the real curves quite well. The simulated jacket temperature rises in the beginning, as does the real jacket temperature, but then, during the time interval of 0.3–0.7 time units, it does not fall far enough compared to the real jacket temperature. This error, in turn, affects all the other variables in this time interval: the simulated reactor temperature is somewhat lower than the real one, the simulated pressure is somewhat higher than the real one, and there are twitches in the simulated concentrations c_{EO} and c_{EC} which are not present in the real concentrations. This error is possibly due to two major things: first, in the simulations we use constant PID parameter values instead of time variable ones, and second, the heat transfer between the reactor content and the jacket water is deliberately modeled with rather low accuracy. In this work, the focus has been on making a simple model to use as a start for further modeling work, and this is why we have chosen to use these approximated values. The relation between the effects of the approximations is difficult to say anything about without further information. In the future, these things should be looked further into.

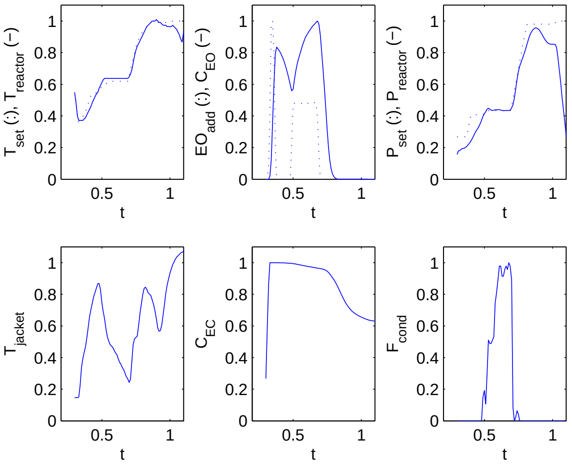


Figure 4: The figure shows real data from the process.

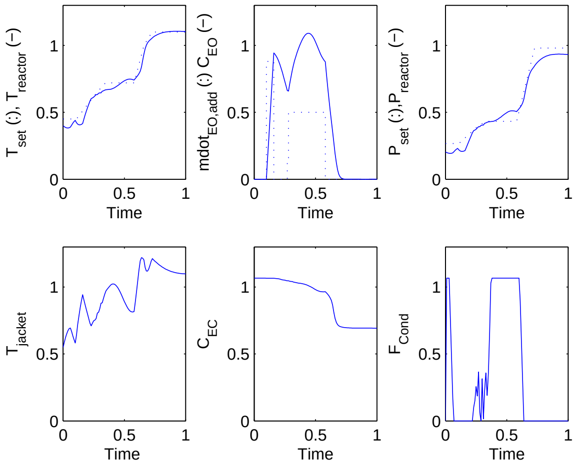


Figure 5: The figure shows a simulation in Simulink using the model equations above. As can be seen, all simulated curves but the jacket temperature follow the real curve quite well.

2.3 Optimization problem

We want to minimize the total batch time and hence use the complete model above to formulate the dynamic minimum time problem, Equation (2). It has the form

$$\begin{aligned} &\text{minimize} && t_f, \\ &\text{subject to} && h(\dot{x}(t), x(t), u(t), t) = 0, \\ &&& g(x(t), u(t), t) \leq 0, \\ &&& x \in X, u(t) \in U, \\ &&& x(0) \in X_0, x(t_f) \in X_f, \\ &&& t \geq 0. \end{aligned}$$

In this study, we consider the reactions starting with the addition of ethylene oxide, including the heat transfer from the reactor, but not loading, preheating, cooling and emptying. We define the end of the batch as the time t_f characterized by the concentration of EC dropping below a limit c^0_{EC}. We optimize the operation by finding an optimal way of adding the ethylene oxide to the reactor, $\dot{m}_{EO}(t)$.

In this formulation, the system equations h are given by the model equations above, summarized as

$$\begin{aligned}
\dot{T}_r &= f_1(T_r, n_{EO}, n_{EK}, n_{RO^-}, T_j, F_c, \dot{m}_{EO}, t),\\
\dot{T}_j &= f_2(T_r, n_{EO}, n_{EK}, n_{RO^-}, T_j, \dot{m}_{EO}, t),\\
\dot{F}_c &= f_3(T_r, n_{EO}, n_{EK}, n_{RO^-}, F_c, \dot{m}_{EO}, t),\\
\dot{n}_{EO} &= f_4(T_r, n_{EO}, t, \dot{m}_{EO}),\\
\dot{n}_{EK} &= f_5(T_r, n_{EK}, n_{RO^-}, t),\\
\dot{n}_{RO^-} &= f_6(T_r, n_{EK}, n_{RO^-}, t),
\end{aligned}$$

with the constraints g (both technical and natural)

$$\begin{aligned}
&0 \le T_r,\\
&c \le T_j \le C,\\
&m \le \frac{\partial T_j}{\partial t} \le M,\\
&0 \le F_c \le D,\\
&l \le \frac{\partial F_c}{\partial t} \le L,\\
&0 \le n_{EO} \le n_{EO,max},\\
&0 \le n_{EK} \le n_{EK,max},\\
&0 \le n_{RO^-} \le n_{RO^-,max}.
\end{aligned}$$

The function $\dot{m}_{EO}(t)$ is parameterized by dividing the batch time into $J = 150$ equal time elements and assuming the flow rate to be constant in each of these elements. To prevent too fast changes in flow rate (which originates from limited capability of pumps etc.), two adjacent elements are not allowed to differ more than a preset value, α:

$$\begin{aligned}
\dot{m}_{EO}(t) &= m_j, \quad t \in [t_{j-1}, t_j),\ j = 1, \dots, J\\
|m_j - m_{j-1}| &\le \alpha, \quad j = 2, \dots, J.
\end{aligned}$$

To prevent too high temperatures and too large temperature gradients, which are not allowed in the real process, but are accepted by MATLAB in simulations, a penalty is added to the objective function:

$$f_{obj} = t_f + P. \tag{6}$$

As a first step, used in the simulations below, a discontinuous penalty is used, namely

$$P(T_r) = \begin{cases} p, & |T_{set} - T_r| \ge \beta,\\ 0, & \text{otherwise}, \end{cases} \tag{7}$$

where $p \gg 0$. It should be mentioned that when performing an automatic optimization, a continuous penalty is preferred, for instance the following

$$P(T_r) = p \max\{0, |T_{set} - T_r| - \beta\}. \tag{8}$$

The penalty P is added in those simulations where the control system does not manage to keep the reactor temperature close enough to the set point temperature T_{set}. The constant β is determined by the ability of the PID controllers to control the reactor temperature and using a large value means that we rely on the jacket to be good at controlling the reactor temperature. Since a DAE system is just a model of the real system, it contains errors, and the constant β is also used as an additional error control of the reactor heat transfer and the control system. If the error in the control system and/or the reactor heat transfer is large and the simulated system is able to control the reactor temperature, a small value of the constant β in Equations (7) and (8) decreases the risk of escalating reactor temperature in the real reactor.

3 Simulations

In this study, the focus has been on finding a mathematical model for the batch time, and initially not on the quality of the end product. Still, we need to use information about the end product quality to determine which profiles are acceptable: if a large portion of the EO is added prior to the wanted reaction temperature is reached, this may result in a worsened product quality. Below, this is judged by the user. Since, prior to this study, there is a lack of knowledge about how the quality is affected by different temperature profiles, adding this to the mathematical model would have been to comprehensive. The acceptable size of the portion of EO added prior to the wanted reaction temperature and how the quality is affected by the reaction temperature are interesting future research topics. To get a proper objective function, the quality should be added to the optimization problem, for instance as a penalty in the objective function just as large temperature gradients above.

Below we use the objective function defined by Equation (6), including a discontinuous penalty according to Equation (7) with $p = 10$. This means that an objective function value above 10 has been penalized. For the original EO profile in Figure 4, this objective function value is $f_{obj} = 0.61$.

A series of simulations have been run, and in each step we change as little as possible, to clearly notice the effects. We compare each simulation with the original profile used in the process today. All simulations have in common that the slopes and the plateau values of the set point curves T_{set} and P_{set} are the same as in the original profile. The starting time for the second set point rise is determined by the end of the EO addition. A reason for not allowing changes in slopes for the set point curves, is that if the reactor temperature (or pressure) rises too fast, there is a potential risk for escalating reactor temperature, which is not wanted; it is even dangerous. Of course, varying the set point curves would be interesting to include in a future optimization with a more accurate model.

We have relaxed the starting times for the first rise of the set point curves by delaying the start of the EO addition, and have run the following series of simulations with piecewise constant EO-profiles:

1. Using an EO-profile with only one plateau, at a starting level being the same as the second plateau in the original profile, varying the delay and level.
2. Using the original EO-profile with two plateaus, varying the levels proportionally and varying the delay.
3. Using a profile with three plateaus varying only the delay.

Table 1: Objective function values for different simulations, with one, two or three plateaus and varying levels and delays.

Delay	**One plateau** Level rise $l = \frac{New\ levels}{Original\ levels}$				**Two plateaus (original profile)** Level rise $l = \frac{New\ levels}{Original\ levels}$									**Three plateaus**
(time units)	1.00	1.20	1.60	2.00	1.00	1.10	1.20	1.30	1.40	1.50	1.60	1.70	1.75	
0.00	0.57	0.56	10.58	10.55	0.61	0.60	0.58	0.58	0.58	0.58	0.58	0.58	10.58	0.55
0.05	0.60	0.57	10.62	10.58	0.65	0.63	0.62	0.62	0.62	0.61	0.61	0.60		0.60
0.10	0.63	0.60	10.62	10.62	0.69	0.68	0.66	0.66	0.66	0.64	0.64	0.62		0.63
0.15	0.67	0.64	0.64	10.65	0.74	0.72	0.71	0.71	0.69	0.68	0.68	0.66		0.65
0.20	0.71	0.68	0.68	10.69	0.78	0.77	0.75	0.75	0.73	0.72	0.72	0.70		0.69
0.25	0.76	0.72	0.72	10.73	0.83	0.81	0.80	0.79	0.78	0.76	0.76	0.74		

4 Results

The different objective values for combinations of variations in delay and variations in levels are shown in Table 1. Using a profile with one plateau as in Figure 6, it is seen that for those simulations in which the penalty is not activated, the batch time decreases with increasing levels, which is natural since higher concentrations of EO in the reactor results in a higher reaction rate according to the reaction rates. But increasing the EO-addition too much results in a too large heat production for the control system to handle, which is seen in that the objective function value is penalized and $f_{obj} > 10$. For each level rise, increasing the delay naturally increases the batch time. For the two smallest level rises (1.00 and 1.20) some of the batch times are smaller than the original profile. However, here the quality must be taken into account, since a portion of the EO is added prior to the reactor temperature reaches the wanted reaction temperature.

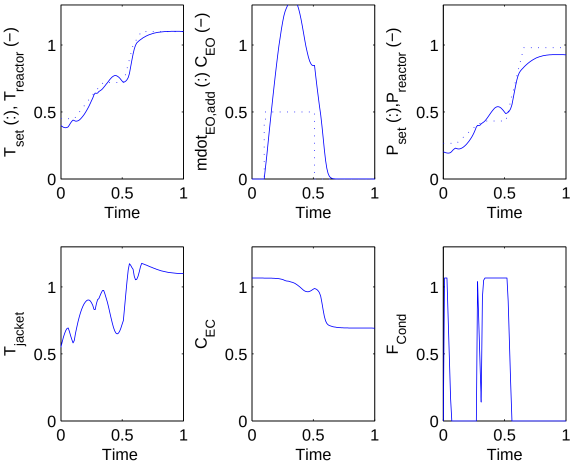


Figure 6: The figure shows a simulation where EO is added at a constant level being the same as the second plateau level in the original profile, with no delay.

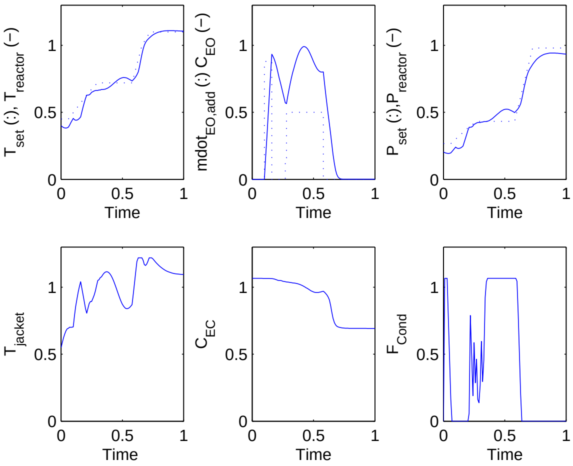
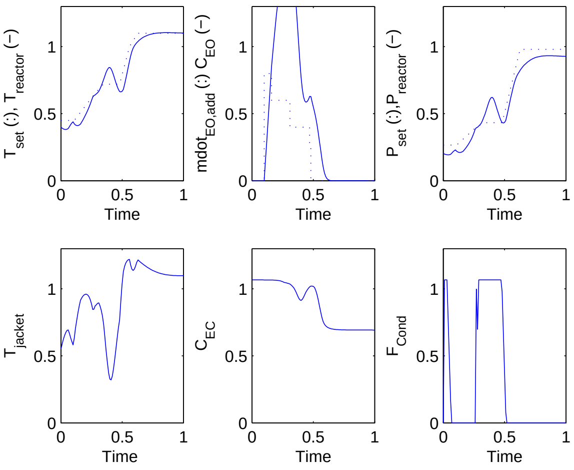


Figure 7: The figure shows a simulation with original EO profile, but where the EO addition is delayed 0.05 time units. The corresponding objective function value is $f_{obj} = 0.65$.

Using variations of the original EO-profile with two plateaus, it can be seen in Table 1, that using a 20 % rise in the plateau levels, with the delay = 0.00, it is possible to shorten the batch time to 0.58 time units, which is an improvement of 5 % compared to the original profile. As mentioned above, in these simulations we have kept the original set point curves. According to these simulations, with no delay, nothing is gained by raising the levels further. We conclude that the batch time increases when delaying the original profile. Figure 7 shows a simulation using the original profile with 0.05 time units delay, with the objective function value $f_{obj} = 0.65$.

Using the profile with three plateaus, again keeping the original set point curves, as in Figure 8, it is possible to decrease the batch time, with delays up to 0.05 time units, which correspond to 10 %. However, also here one must keep the quality in mind; in order to to determine whether these profiles give acceptable quality, more research is needed.



Figur 8: The figure shows a simulation in which the EO-profile has tree plateaus and no delay.

Summarizing, we have used piecewise constant EO profiles with up to three constant plateaus and varying levels, and simulations show that a 5 % increase in total batch time is possible, using a profile with two plateaus as in the original, but with 20 % higher levels and no delay.

Even a 10 % shorter batch time than today is possible, using a profile with three different plateau levels. However, in this profile, a large portion of the EO is added prior to when the wanted reaction temperature is reached, which may result in a worsened end product quality. In order to decide which profiles are acceptable, more research about the effect of the reaction temperature used on the end product quality is needed.

5 Future work

When optimizing the operation of a semi-batch reactor, an overall point of view is advantageous, since the decisions are of an economic character: mainly the costs of raw material, the production, and the end product quality. This should be kept in mind when performing an optimization like in this work. Shortening the batch time with for instance 10 % may in the end not decrease the total cost with more than 0.5 %.

This work is the first step in optimizing the operation of a semi-batch reactor. Steps planned to be followed include improving the process model, extending the optimization problem, performing the optimization with the aid of CVP and testing the optimal solution in the real process. We also intend to look further into other optimization techniques, such as simultaneous methods and optimization under uncertainty.

Work on improving the process model has already started, especially on achieving better values for the heat capacity of the reactor content $C_{P,tot}$. In the future, also a more complete model of the jacket system is to be added to the optimization problem. Several parameters in the model used in this work are uncertain to different degrees. Including uncertainty into the process model gives a different type of optimization problem, which demands other optimization techniques than discussed in this study [8, 11, 15, 16, 17].

As a first extension of the optimization problem, we recommend that the quality of the end product is included in the objective function of the optimization problem, following a proper mathematical modeling of this entity. From the series of simulations performed in this work, it is hard to tell which profile is the best. It is highly probable that further investigations, and especially automatic optimization, can show profiles resulting in even shorter batch times.

In an extended optimization problem, both the temperature and the pressure set point curves should be used as control variables and hence optimized over, together with the addition of the EO. The impact of the different set point curves on the total batch time in optimization is interesting to study, since the batch time depends on the reaction rates, which in turn strongly depend on the temperature. The pressure is strongly connected to the temperature due to the gas phase present and the chosen working point.

Performing a complete optimization to find a solution to the dynamic optimization problem, using for instance the control vector parametrization approach for the solution, can give useful, and perhaps unexpected, profiles. In parallel to improving the model, we intend to use the existing model when using CVP to optimize the operation of the process.

We already know that our existing model contains uncertainty, and the sensitivity of input parameters must be further investigated before the optimal solution is tested in the real process. An investigation into these uncertainties and their effects may ultimately produce a new and more robust optimization formulation of the problem. This work is also ongoing in parallel to the above mentioned work.

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Nomenclature

m_i = mass of substance i, kg
M_{EO} = molar mass for EO, kg/mol
T_r = average reactor temperature, K
T_0 = temperature of added EO, K
$\overline{T}_j$ = average jacket temperature, K
$T_{c,in}$ = temperature of water into condenser, K
F_c = water flow through the condenser, m^3/s
P_r = reactor pressure, Pa
$\dot{n}$ = molar flow of EO into the reactor, $mole/min$
n_i = moles of substance i in the reactor, $mole$
c_i = concentration of substance i in the reactor, $mole/m^3$
k_j = heat transfer coefficient from reactor content to jacket water, $W/m^2, K$
k_c = heat transfer coefficient from reactor content to condenser water, $W/m^2, K$
U_c = overall heat transfer coefficient from reactor content to condenser water, $W/m^2, K$
A_j = jacket area, m^2
A_c = condenser area, m^2
A_i = constant in Arrhenius equation for reaction i
E_i = activation energy in Arrhenius equation for reaction i
r = set point
y = measured variable
u = controlled variable
K = proportional constant for regulator
T_I = integral constant for regulator
T_D = derivative constant for regulator

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