

# Technical Report

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## Temperature modelling and Model Predictive Control of a pilot-scale batch reaction system

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## Abstract

The temperature control equipment on a pilot scale batch reaction system located at EAFIT University in Medellín, Colombia, is modeled and a new controller is designed aiming at using it in the reactor current PLC-based control system. Some mathematical models are developed from experimental data to describe the system behavior and using them several model based predictive controllers are designed. The simplest, yet reliable, model obtained is an ARX polynomial model of order (1,1,1) that yields a four states affine model for which an explicit MPC was calculated. This controller has a reduced mathematical complexity and can probably be used directly on the existing control system.

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## 1 Introduction

The Department of Process Engineering at EAFIT University in Medellín, Colombia, has among its resources an important equipment for studying batch processes consisting of a robust and versatile pilot scale batch reaction system. However, because of several past events it had been non-operative for some time until a recent project rehabilitated it, reconstructing its control system and updating its documentation; making it suitable for operation once again. This was done looking forward to improving the teaching and researching capabilities of the institution in the area of discontinuous chemical processes. The intention is to develop laboratory experiences and complementary activities contributing to the formation of students and the materialization of research initiatives. Among the control system needed to be implemented in order to achieve this goal is the temperature control loop. This loop should maintain the temperature inside the reaction vessel close to a reference value by manipulating some elements on the system.

To accomplish this a model based control strategy is considered because this kind of strategies have had a significant impact in industrial application due to their ability to tackle complex problems, optimizing the behavior of the plant by using a dynamical model to predict its response to the control signals and thus selecting the best value for them according to the objectives defined.

To carry forward this development a research proposal was formulated for a short academic visit to IRI and this was funded by the 2013–2014 Becas Iberoamérica Jóvenes Profesores e Investigadores Scholarship by Santander Universidades. This document presents the development and results of the activities carried out. First, a short functional description is presented in order to clarify the structure of the physical system and establish some guidelines for its modeling. Then some mathematical models formulated for the system are presented, one of them a semi-empirical model based on the phenomenon and other one an ARX polynomial model. Using this models some model based controllers are constructed and from the simplest one an explicit MPC is formulated. Finally, some tests are performed and some conclusions are drawn.

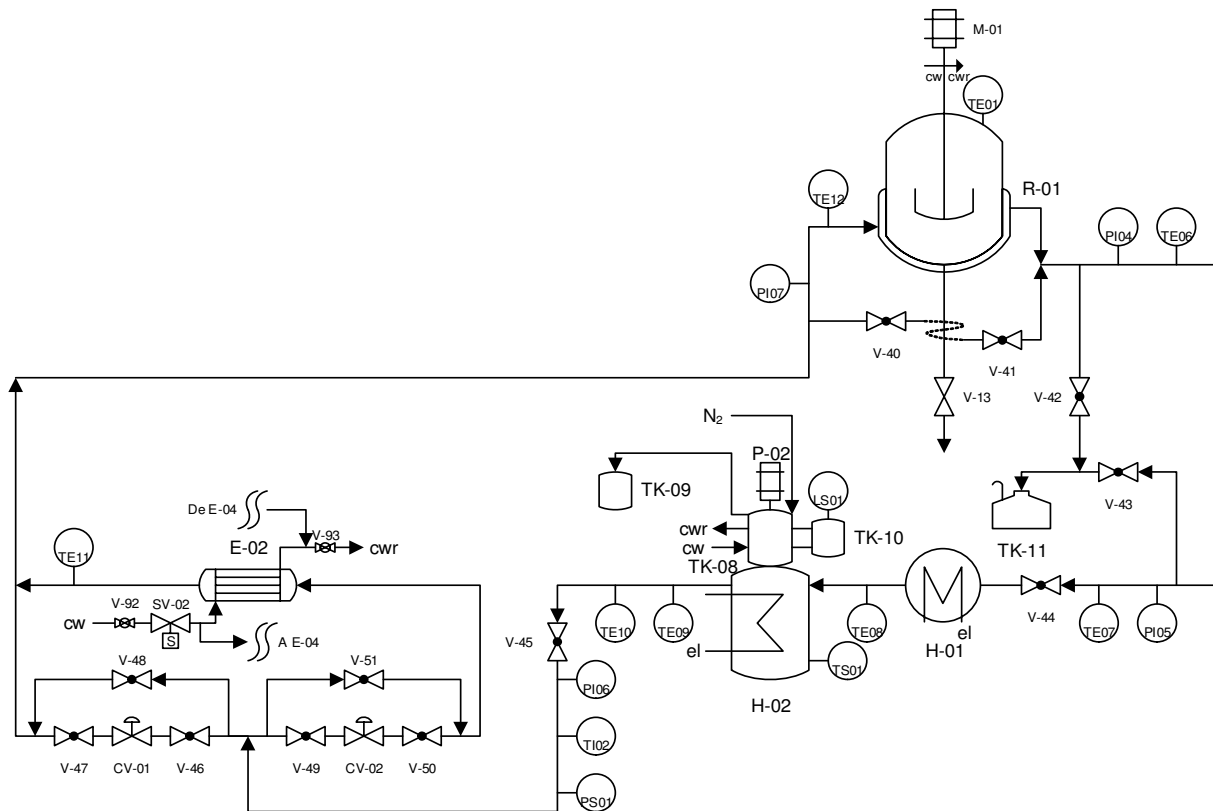
## 2 System Description

The temperature control equipment studied consists of a thermal fluid circuit that supplies the required thermic energy to the reaction vessel or removes surplus heat according to process needs. A process flow diagram –PFD– for this system is presented in Figure 1.

The thermal fluid is heated by a couple of electrical resistance heaters (H-01, H-02) and pumped by P-02. The fluid then flows through pipeline towards the jacketed reaction vessel and back to the heaters. Along the way there are several elements, such as valves and temperature/pressure instruments, that allow the measurement of some variables and the manipulation of flow.

After leaving the heaters/pump the fluid goes to the jacket through one of two paths: the first one delivers it directly while the other one passes through a heat exchanger where the fluid can be cooled when necessary by means of cooling water. Thus, the action of heating the fluid is accomplished by turning on the electrical resistances inside the heaters and cooling is reached by enabling the flow through the cooling water heat exchanger (E-02).

The temperature after thermal fluid heating is measured by instrument TE-10 and before entering the vessel's jacket is measured by TE-12. At the exit of said jacket there is TE-06 and TE-07 is placed before entering the heaters. The controlled variable is the temperature of the reacting mixture inside the vessel, measured by TE-01.



**Figure 1:** PFD for the analyzed system

### 3 Phenomenological-based Model

According to the previous description the system can be divided into three control volumes for its study:

- The reaction vessel, where the transfer between the thermal fluid and the reaction mixture, through the jacket, takes place to supply or remove the required energy. It will be referred to with the subscript  $j$ .
- The piping and equipment between the exit of the vessel jacket and the exit of the fluid pump/heater (H-02). This section is limited between TE-06 and TE-10 and will be referred to as  $p_1$ . Here the thermal fluid is heated by electrical resistances and some loss to the environment occurs.
- The piping between the exit of the fluid pump/heater and the inlet to the vessel jacket. Delimited by TE-10 and TE-12. Referred to as  $p_2$ . Some loss to the environment occurs and the thermal fluid cooler, which accounts for the fluid cooling when the required action is to cool down the vessel, can be included here too as an additional exchanger with the subscript  $c$ .

In general, all these sections can be modeled from the general energy balance

$$\text{Input} + \text{Generation} = \text{Output} + \text{Acumulation}. \quad (1)$$

From which particular equations can be written for each section considering the phenomena taking place in each one. The terms considered are described next.

**Input.** Energy content of the fluid stream entering the control volume. Given by its enthalpy, i.e.,

$$I_i = \dot{H}_{in} = \int_{T_{ref}}^{T_{in}} \dot{m} C_p dT. \quad (2)$$

This, considering constant specific heat capacity and taking  $0^\circ C$  as the reference temperature, gives:

$$I_i = \dot{m} C_p T_{in}. \quad (3)$$

**Generation.** Energy generated inside the control volume. It occurs only within the heaters and the value is given by the power of the electrical resistances used, i.e.,

$$G_{p_1} = \dot{Q}_R. \quad (4)$$

**Output.** This one have two components. Energy content of the fluid stream leaving the control volume. Given, again, by its enthalpy:

$$O_i = \dot{m} C_p T_{out}. \quad (5)$$

And the energy exchange with the environment, the materials inside the reaction vessel or the cooling water in E-02, all of those estimated by treating each section as a heat exchanger, i.e.,

$$O_i = U A_i LMTD_i. \quad (6)$$

Here, the global heat transfer coefficient ( $U$ ) is a numerical value that encompasses the different mechanisms involved and is a function of many factors, which makes it very difficult to calculate from a phenomenological approach. Besides, considering the complex geometry of the elements involved, it is much preferable to group the factors  $U$  and  $A$  and estimate  $UA_i$  for each section from experimental data.

The temperature difference for this energy exchange can be calculated as the *Log Mean Temperature Difference* – $LMTD$ –, since the characteristics of this phenomenon are very similar to those of a heat exchanger. The expression for  $LMTD_i$ , which accounts for the fact that the temperature difference along a heat exchanger is not constant, is:

$$LMTD_i = \frac{(T_{in} - T_{\infty}) - (T_{out} - T_{\infty})}{\ln\left(\frac{T_{in} - T_{\infty}}{T_{out} - T_{\infty}}\right)}. \quad (7)$$

$T_{in}$  and  $T_{out}$  are the temperature of the fluid coming in, and going out, the control volume. And  $T_{\infty}$  is the temperature of the medium which the exchange is performed with.

**Accumulation.** Change in the thermal energy stored within the control volume,

$$A_i = \frac{d(m Cp T)}{dt}. \quad (8)$$

which, considering the amount of fluid inside the control volume as constant; as well as the specific heat capacity. And if this temperature is taken as the mean between inlet and outlet temperatures on each section, gives:

$$A_i = \frac{m_i Cp}{2} \left( \frac{dT_{in}}{dt} + \frac{dT_{out}}{dt} \right), \quad (9)$$

where  $m_i$  refers to the amount of thermal fluid inside each control volume.

This general analysis, applied to each one of the defined control volumes, yields:

- For the first piping section, carrying the thermal fluid from the jacket and through the heaters:

$$\dot{m} Cp T_{06} + \dot{Q}_R = \dot{m} Cp T_{10} + UA_{p1} LMTD_{p1} + \frac{m_{p1} Cp}{2} \left( \frac{dT_{06}}{dt} + \frac{dT_{10}}{dt} \right). \quad (10)$$

- For the second piping section, from the heaters to the vessel jacket, and trough the cooler in such a case:

$$\dot{m} Cp T_{10} = \dot{m} Cp T_{12} + UA_{p2} LMTD_{p2} + UA_c LMTD_c + \frac{m_{p2} Cp}{2} \left( \frac{dT_{10}}{dt} + \frac{dT_{12}}{dt} \right). \quad (11)$$

- For the thermal fluid passing through the vessel jacket:

$$\dot{m} Cp T_{12} = \dot{m} Cp T_{06} + UA_j LMTD_j + UA_e LMTD_e + \frac{m_j Cp}{2} \left( \frac{dT_{12}}{dt} + \frac{dT_{06}}{dt} \right). \quad (12)$$

In addition, the materials inside the reaction vessel must be considered too. This is, in this case, a closed system since no mass leaves or enter the vessel. There is no generation and the only energy entry is the heat transferred through the vessel jacket. This leaves

$$UA_j LMTD_j = UA_R \Delta T_R + m_R C_{pR} \frac{dT_{01}}{dt}, \quad (13)$$

where, considering the temperature inside the vessel ( $T_{01}$ ) and the temperature of the environment ( $T_e$ ) are uniform, i.e.,

$$\Delta T_R = T_{01} - T_e. \quad (14)$$

These equations can be rearranged to obtain the expressions for  $\frac{dT_i}{dt}$  as

$$\frac{dT_{10}}{dt} = \frac{2 \left( \dot{m} C_p T_{06} + \dot{Q}_R - \dot{m} C_p T_{10} - UA_{p1} LMTD_{p1} \right)}{m_{p1} C_p} - \frac{dT_{06}}{dt}, \quad (15)$$

$$\frac{dT_{12}}{dt} = \frac{2 \left( \dot{m} C_p T_{10} - \dot{m} C_p T_{12} - UA_{p2} LMTD_{p2} - UA_c LMTD_c \right)}{m_{p2} C_p} - \frac{dT_{10}}{dt}, \quad (16)$$

$$\frac{dT_{06}}{dt} = \frac{2 \left( \dot{m} C_p T_{12} - \dot{m} C_p T_{06} - UA_j LMTD_j - UA_e LMTD_e \right)}{m_j C_p} - \frac{dT_{12}}{dt}, \quad (17)$$

$$\frac{dT_{01}}{dt} = \frac{UA_j LMTD_j - UA_R \Delta T_R}{m_R C_{pR}}, \quad (18)$$

where,

$$LMTD_{p1} = \frac{(T_{06} - T_e) - (T_{10} - T_e)}{\ln \left( \frac{T_{06} - T_e}{T_{10} - T_e} \right)}, \quad (19)$$

$$LMTD_{p2} = \frac{(T_{10} - T_e) - (T_{12} - T_e)}{\ln \left( \frac{T_{10} - T_e}{T_{12} - T_e} \right)}, \quad (20)$$

$$LMTD_c = \frac{(T_{10} - T_{cw}) - (T_{12} - T_{cw})}{\ln \left( \frac{T_{10} - T_{cw}}{T_{12} - T_{cw}} \right)}, \quad (21)$$

$$LMTD_j = \frac{(T_{12} - T_{01}) - (T_{06} - T_{01})}{\ln \left( \frac{T_{12} - T_{01}}{T_{06} - T_{01}} \right)}, \quad (22)$$

$$LMTD_e = \frac{(T_{12} - T_e) - (T_{06} - T_e)}{\ln \left( \frac{T_{12} - T_e}{T_{06} - T_e} \right)}, \quad (23)$$

$$\Delta T_R = T_{01} - T_e. \quad (24)$$

where  $\dot{m}$  and  $\dot{Q}_R$  are inputs to the model. And  $UA_{p1}$ ,  $UA_{p2}$ ,  $UA_c$ ,  $UA_j$ ,  $UA_e$  and  $UA_R$  are parameters determined from experimental data. A complete list of the symbols used is available in the Appendix.

Unfortunately, suitable values for the parameters could not be found from the experimental data available. Thus a different approach had to be taken and this phenomenological-based model remains an open question for future work.



## 4 ARX Model

Similarly to the last section some control volumes are defined to describe the system:

- The reaction vessel, where the reaction mixture is contained and the reaction takes place. Its temperature,  $T_{01}$ , is influenced by the transfer from the thermal fluid, the loss to the environment and the reaction consumption. It will be referred to with the subscript  $R$ .
- The reaction vessel jacket, where the transfer between the thermal fluid and the reaction mixture takes place to supply or remove the required energy. It will be referred to with the subscript  $j$  and is limited between TE-12 and TE-06.
- The piping and equipment between the exit of the vessel jacket and the exit of the fluid pump/heater (H-02). This section is limited between TE-06 and TE-10 and will be referred to as  $p_1$ . Here the thermal fluid is heated by electrical resistances and some loss to the environment occurs.
- The piping and equipment between the exit of the fluid pump/heater and the inlet to the vessel jacket. Delimited by TE-10 and TE-12. Referred to as  $p_2$ . Some loss to the environment occurs and the thermal fluid cooler, which accounts for the fluid cooling when the required action is to cool down the vessel, is placed here.

The measured temperatures are, accordingly,  $T_{01}$ ,  $T_{06}$ ,  $T_{10}$  and  $T_{12}$ ; being  $T_{01}$  the output whose behavior is intended to be controlled. The manipulated inputs are heating and cooling of the thermal fluid accomplished by turning on the electric heaters or diverting the fluid flow through E-02 by using CV-01 and CV-02. These valves can also regulate the volume flow of fluid since they are pneumatic proportional valves. Nevertheless, due to the preliminary character of this work and obstacles for measuring this flow and determining simple parameters to include it on the model, it was decided to fix the valve openings to 90% and flow variation will be subject to future work. As seen before, on an early stage of the system modeling a phenomenological model was proposed, but due to difficulties on the estimation of its parameters a different approach had to be taken. The models used for the simulation of the system and the computing of MPC are now described.

In general, the temperature of a body is nothing more than an expression of the amount of thermic energy it contains. So, given that the thermic energy in any point of the subject system at a given time depends on the energy it had on previous instants and the energy inputs or outputs affecting it, the temperature at any point can be modelled as a function of the previous temperature and the variables affecting its energy content. This way ARX models can be used, obtaining its coefficients from experimental data.

These ARX models are linear difference equations of the form

$$A(z)y(t) = B(z)u(t) + e(t), \quad (25)$$

with the vectors  $A(z)$  and  $B(z)$  containing coefficients according to the desired order for the model [6].

To obtain these coefficients a set of experimental data was processed using MATLAB's *System Identification Toolbox* [5] and a suitable set of models for the considered variables was produced.

For the first control volume, the reaction vessel, the output variable is the temperature of the reaction mixture ( $T_{01}$ ). The energy input is given by the transfer from the thermal fluid

passing through the jacket and the energy output is caused by the loss to the environment. Both energy transfers are driven by the temperature difference between the measured temperature and the corresponding fluid –thermal fluid for the input and environment air for the output– and thereby these temperature differences are the model inputs.

The temperature difference is calculated as the *Log Mean Temperature Difference* –LMTD–,

$$LMTD_i = \frac{(T_{in} - T_{\infty}) - (T_{out} - T_{\infty})}{\ln \left( \frac{T_{in} - T_{\infty}}{T_{out} - T_{\infty}} \right)}, \quad (26)$$

whereas, for the loss to the environment the simple temperature difference is used since in this case both temperatures –mixture and environment– are uniform. Thus  $\Delta T_R = T_{01} - T_e$ .

This way, for the first model  $y(t) = T_{01}(t)$  and  $u(t) = \{LMTD_j(t), \Delta T_R(t)\}$ , yielding

$$A_R(z)T_{01}(t) = B_R(z)_{\{1\}}LMTD_j(t) + B_R(z)_{\{2\}}\Delta T_R(t). \quad (27)$$

The main difference between this one and the remaining control volumes is that those are “open” control volumes in the sense that there is a flow coming in and out its limits. As a result, the temperatures of the incoming fluids are additional inputs in the calculation of the outlet temperatures, which are those models outputs.

For the reaction vessel jacket equation, the output is then the temperature of fluid leaving it ( $T_{06}$ ), measured by TE-06. The inputs are the temperature differences with the reaction mixture, to account for the energy transferred to it, and with the surrounding air to account for the loss to the environment; in addition to the temperature of the fluid coming in,  $T_{12}$ . Thus  $y(t) = T_{06}(t)$  and  $u(t) = \{T_{12}, LMTD_j(t), LMTD_e(t)\}$ . Giving

$$A_j(z)T_{06}(t) = B_j(z)_{\{1\}}T_{12} + B_j(z)_{\{2\}}LMTD_j(t) + B_j(z)_{\{3\}}LMTD_e(t). \quad (28)$$

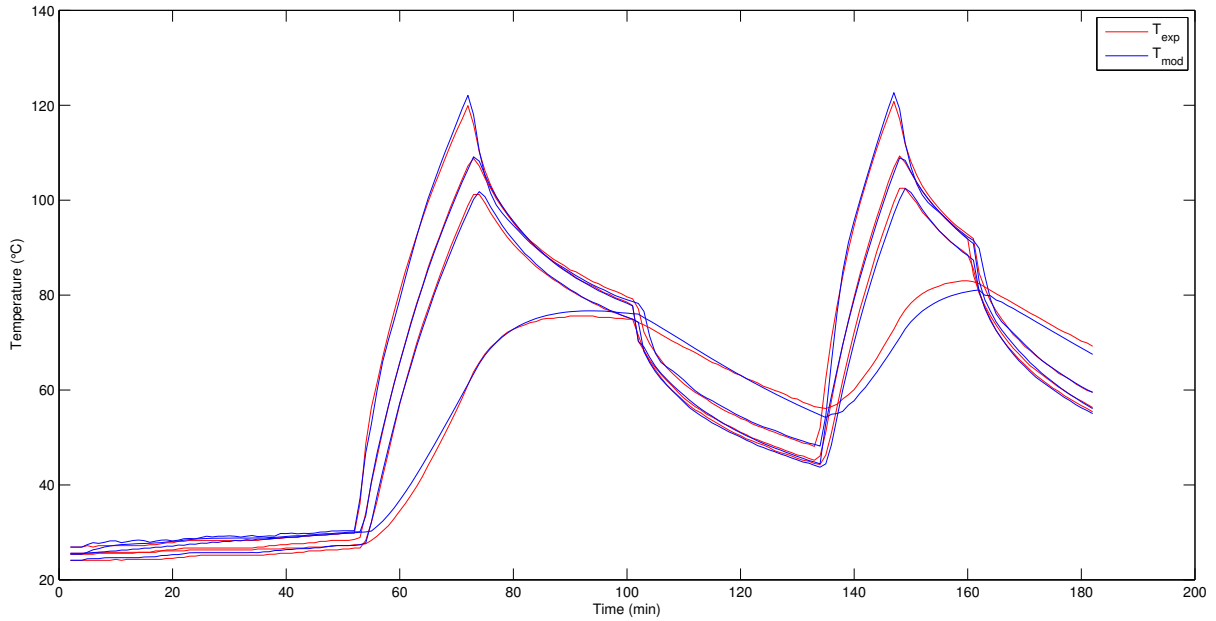
The remaining control volumes have similar characteristics, with the addition of the manipulated inputs of the system as inputs to the models: electric heating ( $H$ ) and cooling ( $cw$ ). Hence,

$$A_{p1}(z)T_{10}(t) = B_{p1}(z)_{\{1\}}T_{06} + B_{p1}(z)_{\{2\}}H(t) + B_{p1}(z)_{\{3\}}LMTD_{p1}, \quad (29)$$

and

$$A_{p2}(z)T_{12}(t) = B_{p2}(z)_{\{1\}}T_{10} + B_{p2}(z)_{\{2\}}cw(t) + B_{p2}(z)_{\{3\}}LMTD_{p2}. \quad (30)$$

As mentioned before, experimental data was analyzed using MATLAB’s *System Identification Toolbox* to compute and validate a set of coefficients to describe the system. In the end, ARX models of order (1,2,1) were obtained for  $p1$  and  $p2$  whereas (1,1,1) was obtained for  $j$  and (1,3,1) for  $R$ . The results are summarized in Figure 2.



**Figure 2:** Experimental data and initial ARX model

## 5 Mathematical model for the MPC

The model presented in the previous section describes in a satisfactory way the system's behavior for simulation, but it poses some inconveniences to the on-line optimization required in an MPC. That's why a simpler model was also developed to ease the aforementioned calculation. This model follows the same structure that the previous one but substitutes the *Log Mean Temperature Difference (LMTD)*, which equation is far from linear, for a simple temperature difference ( $\Delta T$ ).

The reason *LMTD* is used in modelling a heat exchanger is that the temperature difference is not constant along the exchanger. But, since in a ARX model this variation can be absorbed by the calculated coefficients, this change in temperature difference expressions can be made.

The orders of the polynomials obtained are (1,1,1) for  $p_1$ ,  $p_2$  and  $j$ ; and (1,3,1) for  $R$ . This model was validated as well and the results obtained were very much alike those in Figure 2.

By doing this substitution the model becomes linear and it can be represented in the form [6]

$$x(k+1) = Ax(k) + Bu(k) + f, \quad (31)$$

with the states being  $T_{01}(k), T_{01}(k-1), T_{01}(k-2), T_{06}(k), T_{10}(k), T_{12}(k), T_{12}(k-1), T_{12}(k-2)$

and  $f$  is an affine factor given by  $CT_e$ . Inputs are  $H(k)$  and  $cw(k)$ . The matrices are:

$$A = \begin{bmatrix} 1.0834 & 0.3764 & -0.4774 & 0 & 0 & 0.0985 & -0.0789 & -0.0043 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.0351 & 0 & 0 & 0.0982 & 0 & 0.8220 & 0 & 0 \\ 0 & 0 & 0 & 0.1566 & 0.8117 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.3515 & 0.6125 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix},$$

$$B = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 8.5704 & 0 \\ 0 & -1.7350 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}, \quad C = \begin{bmatrix} 0.0035 \\ 0 \\ 0 \\ 0.0116 \\ 0.0724 \\ 0.0619 \\ 0 \\ 0 \end{bmatrix}.$$

Moreover, the outputs are:

$$T_{01}(k+1) = x(k+1)_{\{1\}} \quad (32)$$

$$T_{06}(k+1) = x(k+1)_{\{4\}} \quad (33)$$

$$T_{10}(k+1) = x(k+1)_{\{5\}} \quad (34)$$

$$T_{12}(k+1) = x(k+1)_{\{6\}} \quad (35)$$

With this linear model the computation of the MPC is much faster and more reliable.

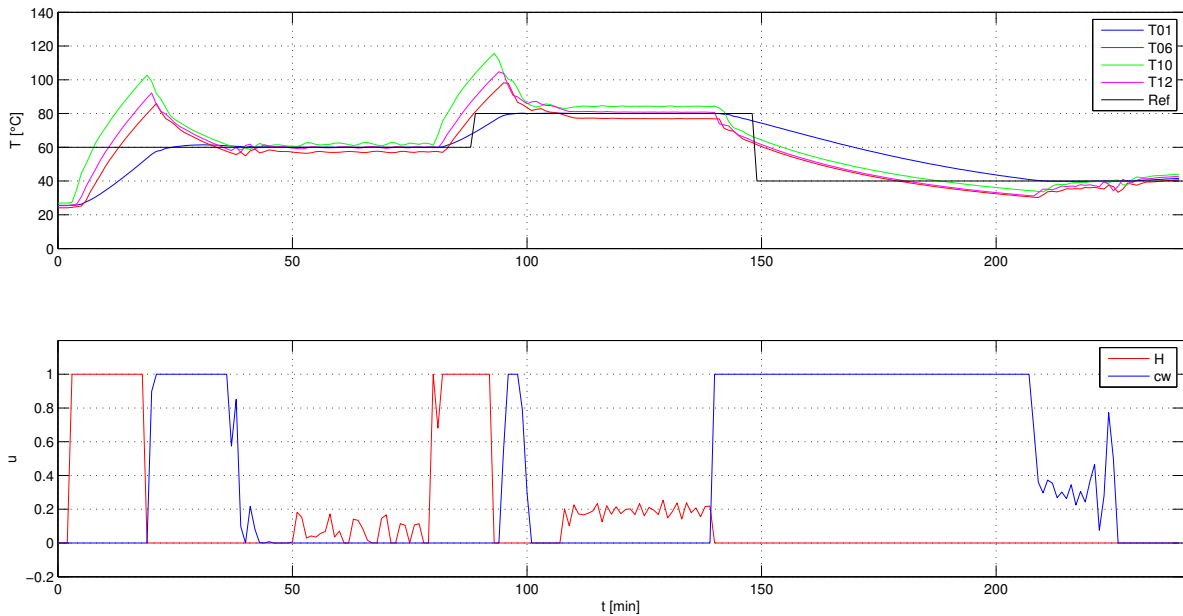
## 6 Preliminary controllers

Using the models described in sections 4 and 5 some preliminary MPC were developed. An hypothetical trajectory was established for the reference temperature, it is fixed at 60 °C during 90 minutes, then it is 80 °C for 60 minutes and finally goes down to 40 °C. This trajectory intends to replicate the one of a typical batch reaction in which the reactants are heated up for mixing, then they are further heated for the reaction to take place and finally they are cooled down for discharge.

The first one of these controllers uses the model from section 4 for both the MPC computation and the system simulation. The optimization problem is solved using MATLAB's `fmincon` function and results are shown in Figure 3. The objective function is of the form

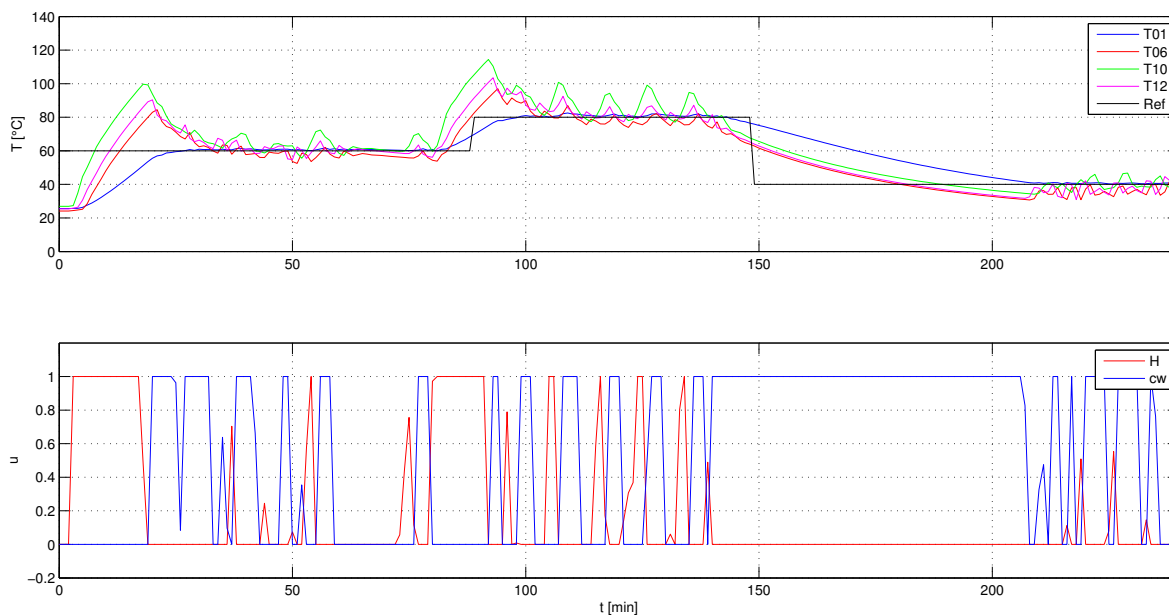
$$J = \gamma_1 \sum_{k=1}^N (T_k - T_k^{ref})^2 + \gamma_2 \sum_{k=1}^N (u_1) + \gamma_3 \sum_{k=1}^N (u_2). \quad (36)$$

For all these preliminary controllers  $H_p = 10$  and  $\gamma_1 = \gamma_2 = \gamma_3 = 1$ . All the calculations were performed on MATLAB R2013b (8.2.0.701) using a Windows 8 PC with Intel CORE i5 3337U, 6 GB RAM. The elapsed time for this controller was 936.89 s.



**Figure 3:** Behavior of preliminary MPC 1: LMTD-LMTD `fmincon`

As presented in Section 5, a simpler model was developed to ease the calculations aiming at the implementation of the final controller on the equipment current PLC-based control system. Figure 4 shows the results obtained using the model from section 5 for the MPC computation and the model from section 4 for the system simulation. The computation took 22.11 s for this simulation, showing the extent of complexity reduction using this simpler linear model.



**Figure 4:** Behavior of preliminary MPC 2: LMTD-131 fmincon

These results show a similar behavior of the controlled variable in both cases but the second controller is more aggressive and uses more of the process inputs to accomplish it. This could be explained by the last model showing a slower response to the inputs.

In order to compare alternatives to solve the optimization problem a different tool was also tested: TOMLAB optimization for MATLAB [4]. Using it under the same conditions as the cases before. Results shown in Figure 5 were obtained after 126.54 s.

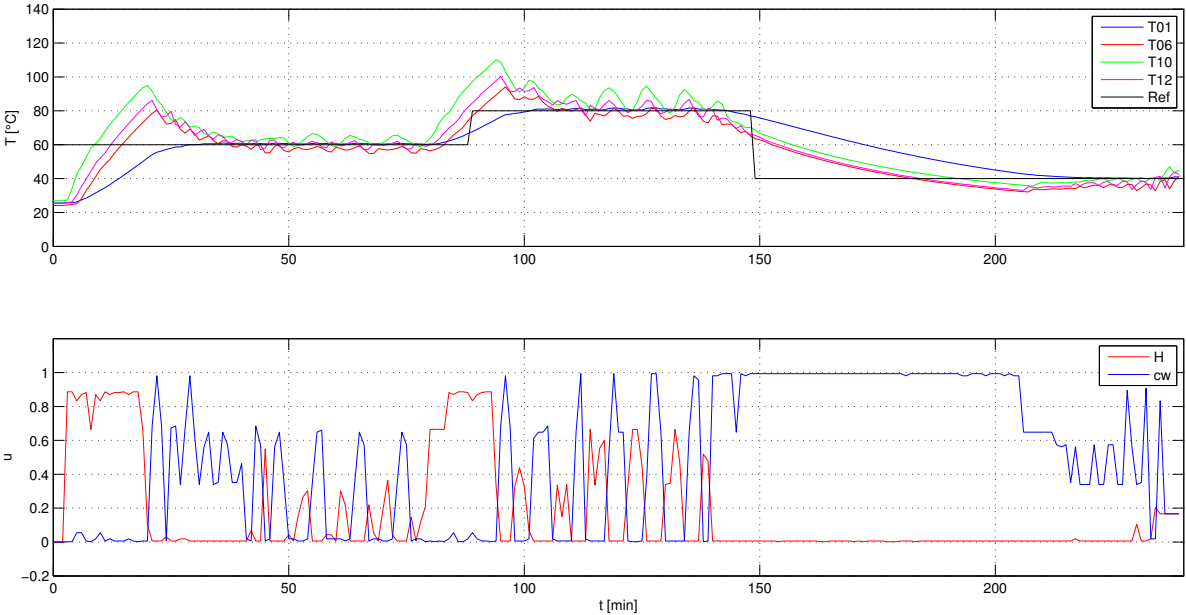
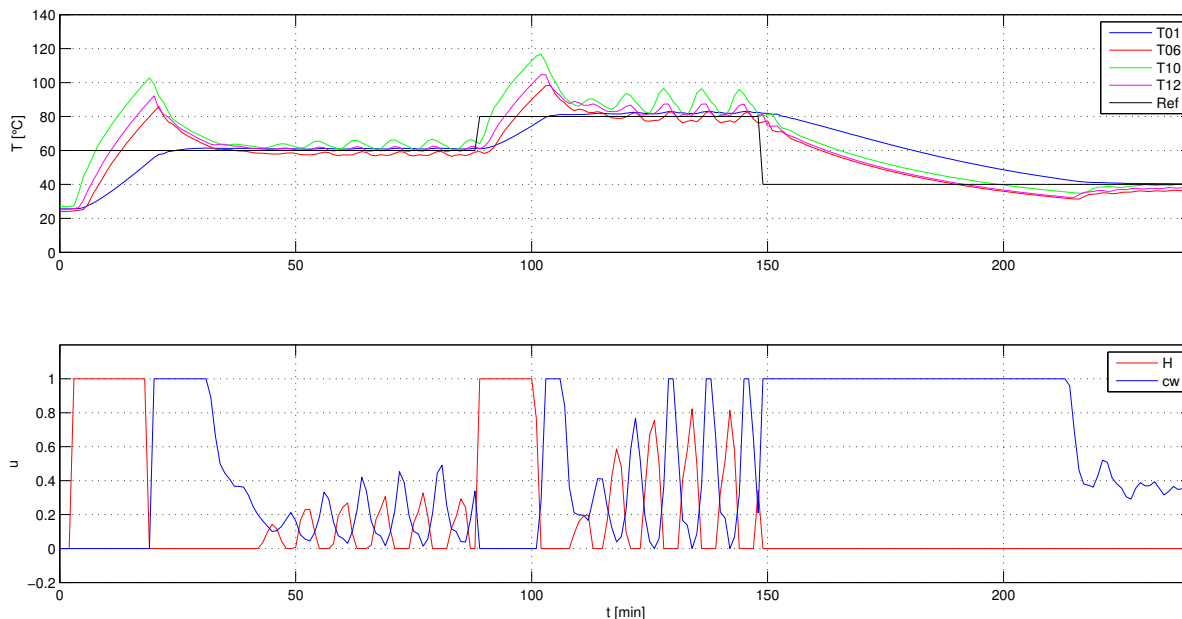


Figure 5: Behavior of preliminary MPC 3: LMTD-131 TOMLAB

Finally, the Multi-Parametric Toolbox 3 (MPT3) [3] was also tested because it offers the option of generating explicit MPC, feature of great interest considering the upcoming step in this work. It took 172.93 s to solve and the results are presented in Figure 6.



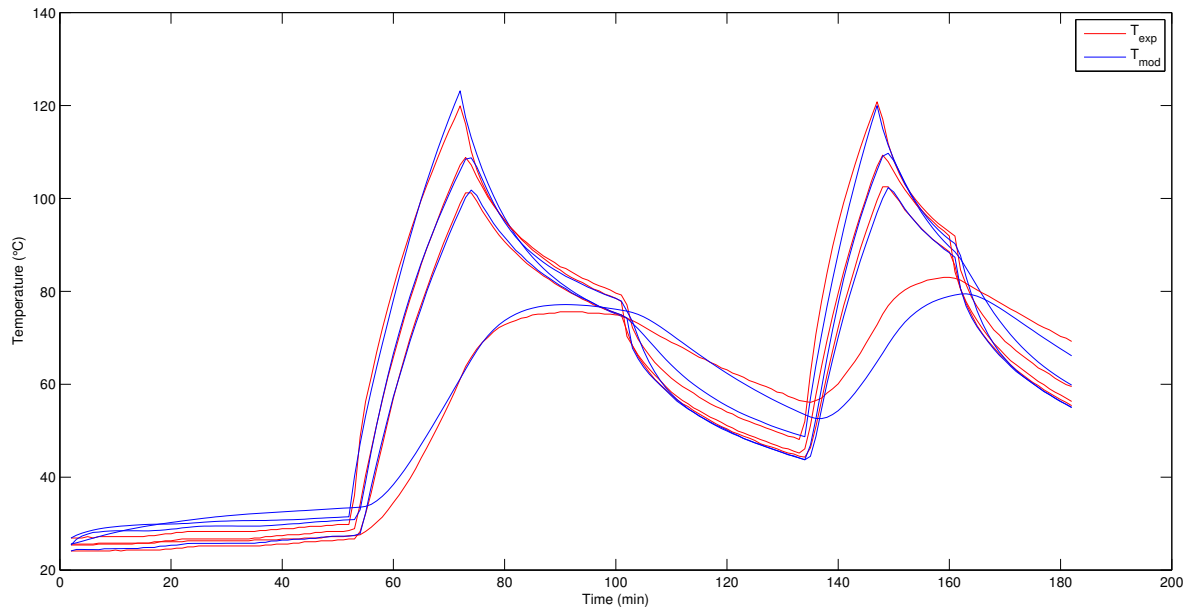
**Figure 6:** Behavior of preliminary MPC 4: LMTD-131 MPT

It can be seen that all these preliminary controllers feature a good reference tracking response, the behavior of the controlled variable is very similar. They all reach the reference value in short time and show little or none overshoot. The main difference between the results using these tools is that `fmincon` and `TOMLAB` are able to “see” the reference shift and thereby they respond prior to it by starting the heating before the reference value shift. This can be seen on the behavior shortly before  $t = 90 \text{ min}$ . On the contrary, MPT does not handle this the same way and in that case heating starts after the reference value shift.



## 7 Explicit MPC

An Explicit MPC was sought looking forward to obtaining a simpler controller suitable to direct calculation by the current PLC on the subject equipment. To attain that the model used in the prediction stage of the MPC was further simplified by reducing the order of the model on section 5 to (1,1,1) for all control volumes. Doing so resulted in a model in the same form as (31) but with just 4 states. The quality of the prediction decreased a little but it is mitigated in the implementation by the feedback from the system measurements. The performance of this ARX model can be seen on Figure 7.



**Figure 7:** ARX model of order (1,1,1) for EMPC

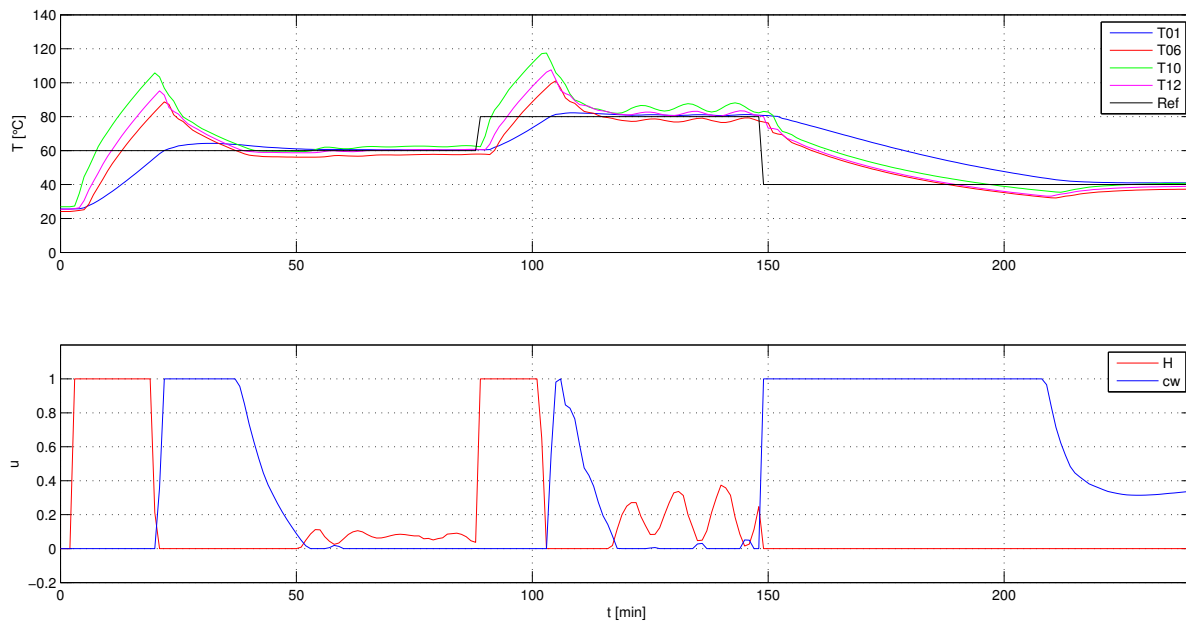
By using MPT3 an EMPC was obtained for the last model, ARX order (1,1,1). The optimization problem is reformulated as a MP-QP –Multi Parametric Quadratic Programming– problem and the state space is divided into several regions when solving and for each one an explicit control law is formulated [2],[1], as follows:

$$u = F_i x + g_i \text{ if } A_i x \leq b_i. \quad (37)$$

In addition, reference tracking can be enabled also by setting the reference as an additional parameter. The solution for this problem, with  $H_p = 5$  to prevent the problem from growing too big, is composed of 38 regions and the results of using it to control the system are shown in Figure 8.

These are very good results, though the reference shifts are not previewed. The controlled variable reaches the reference quickly and with a small overshoot. The changes on input variables are softer than those of on-line optimization solutions and the simple computation of control laws (only matrix sums and products), along with the still manageable number of regions and

size of the matrices involved, makes it possible to think of its direct implementation on the subject equipment.



**Figure 8:** Behavior of preliminary EMPC

## 8 Conclusions

When modelling the behavior of this system ARX models resulted to be a very good alternative to the phenomenological ones originally proposed, which could not be developed due to difficulties on the estimation of its parameters, because the system's physical structure is actually very similar to that of ARX. Considering the temperature of a body is just an expression of the amount of thermic energy it contains and that this amount at a given time depends on the energy it had on previous moments and the energy inputs or outputs affecting it, the value of inputs and current/previous states determines the future value of states and system outputs.

The ARX model of order (1,2,1) obtained for  $p_1$  and  $p_2$ , (1,1,1) for  $j$  and (1,3,1) for  $R$  using MATLAB's *System Identification Toolbox* describes in a satisfactory way the system's behavior for simulation. But since it poses some inconveniences to the on-line optimization required in an MPC a simpler model was also developed to ease the aforementioned calculation. This model follows the same structure that the previous one but substitutes the *Log Mean Temperature Difference (LMTD)*, which equation is far from linear, for a simple temperature difference ( $\Delta T$ ); turning the model into linear. Using this last model the computation of the MPC resulted much faster and more reliable and both *fmincon* and *TOMLAB* obtained satisfactory results on reference tracking for a hypothetical trajectory intended to replicate the one of a typical batch reaction.

The even simpler model – order (1,1,1),  $\Delta T$  – was developed to ease the calculations aiming at the implementation of the final controller on the equipment current PLC-based control system. The results obtained using this model show a similar behavior of the controlled variable to the previous ones but this controller is more aggressive and uses more of the process inputs to accomplish it. This could be explained by this simplified model showing a slower response to the inputs. All these preliminary controllers feature a good reference tracking response and the behavior of the controlled variable is very similar. They all reach the reference value in short time and show little or none overshoot.

The explicit MPC obtained using MPT with the simplest model developed – order (1,1,1) –, is composed of 38 regions and the results of using it to control the system were very good, though the reference shifts are no previewed. The controlled variable reaches the reference quickly and with a small overshoot. The changes on input variables are softer than those of on-line optimization solutions. The main drawback of this last controller is that *fmincon* and *TOMLAB* are able to “see” the reference shift and thereby they respond prior to it by starting the heating before the reference value shift.

The simple computation of control laws (only matrix sums and products), along with the still manageable number of regions and size of the matrices involved, makes it possible to think of the direct implementation of the explicit MPC on the subject equipment. What will be the subject of future work.

## Appendix

The symbols used on this work are:

$C_p$ : Thermal fluid specific heat.

$C_{pR}$ : Specific heat of materials inside the reaction vessel.

$LMTD_c$ : Log mean temperature difference at thermal fluid cooler, between thermal fluid and cooling water.

$LMTD_e$ : Log mean temperature difference at vessel jacket, between jacket and environment.

$LMTD_j$ : Log mean temperature difference at vessel jacket, between thermal fluid and mixture inside the vessel.

$LMTD_{p1}$ : Log mean temperature difference at piping section 1, between piping and environment.

$LMTD_{p2}$ : Log mean temperature difference at piping section 2, between piping and environment.

$LMTD_R$ : Log mean temperature difference at reaction vessel, between vessel and environment.

$\dot{m}$ : Thermal fluid mass flow.

$m_j$ : Thermal fluid mass accumulated within vessel jacket.

$m_{p1}$ : Thermal fluid mass accumulated within piping section 1.

$m_{p2}$ : Thermal fluid mass accumulated within piping section 2.

$m_R$ : Mass of materials inside the reaction vessel.

$\dot{Q}_R$ : Electrical resistances power.

$T_\infty$ : Medium temperature.

$T_{cw}$ : Cooling water temperature.

$T_e$ : Environment temperature.

$T_{01}$ : Temperature at TE-01. Inside the reaction vessel.

$T_{06}$ : Temperature at TE-06. Thermal fluid leaving the vessel jacket.

$T_{10}$ : Temperature at TE-10. Thermal fluid leaving the pump/heater.

$T_{12}$ : Temperature at TE-12. Thermal fluid entering the vessel jacket.

$UA_c$ : General heat transfer coefficient for the thermal fluid cooler.

$UA_e$ : General heat transfer coefficient for the loss to environment in vessel jacket.

$UA_j$ : General heat transfer coefficient for the vessel jacket.

$UA_{p1}$ : General heat transfer coefficient for the loss to environment in piping section 1.

$UA_{p2}$ : General heat transfer coefficient for the loss to environment in piping section 2.

$UA_R$ : General heat transfer coefficient for the loss to environment in reaction vessel.

## References

- [1] A. Bemporad, F. Borrelli, and M. Morari. Model Predictive Control Based on Linear Programming - The Explicit Solution. *IEEE Transactions on Automatic Control*, 47(12):1974–1985, December 2002.
- [2] A. Bemporad, M. Morari, V. Dua, and E.N. Pistikopoulos. The Explicit Linear Quadratic Regulator for Constrained Systems. *Automatica*, 38(1):3–20, January 2002.
- [3] M. Herceg, M. Kvasnica, C.N. Jones, and M. Morari. Multi-Parametric Toolbox 3.0. In *Proceedings of the European Control Conference*, pages 502–510, Zürich, Switzerland, July 17–19 2013.
- [4] Kenneth Holmström. Tomlab – an environment for solving optimization problems in matlab. In *Proceedings for the Nordic MATLAB Conference '97*, pages 27–28, 1997.
- [5] Lennart Ljung. System identification toolbox for use with MATLAB : user's guide, 1995.
- [6] Lennart Ljung. *System Identification: Theory for the User*. PTR Prentice Hall, Upper Saddle River, N.J., 2nd edition, 1999.



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