## Research Article

# Methodology of Supervision by Analysis of Thermal Flux for Thermal Conduction of a Batch Chemical Reactor Equipped with a Monofluid Heating/Cooling System

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We present the thermal behavior of a batch reactor to jacket equipped with a monofluid heating/cooling system. Heating and cooling are provided respectively by an electrical resistance and two plate heat exchangers. The control of the temperature of the reaction is based on the supervision system. This strategy of management of the thermal devices is based on the usage of the thermal flux as manipulated variable. The modulation of the monofluid temperature by acting on the heating power or on the opening degrees of an air-to-open valve that delivers the monofluid to heat exchanger. The study shows that the application of this method for the conduct of the pilot reactor gives good results in simulation and that taking into account the dynamics of the various apparatuses greatly improves ride quality of conduct. In addition thermal control of an exothermic reaction (mononitration) shows that the consideration of heat generated in the model representation improve the results by elimination any overshooting of the set-point temperature.

## 1. Introduction

A large number of industrial processes, such as the production of polymers, fine chemicals, and pharmaceuticals for which continuous production is not feasible or economically attractive, are operated in batch reactor.

In many cases this mode of operation is used to manufacture a variety of products that involve significantly different characteristics such as the conversion time and heat of the reaction. The control of such a type of reactors is completely often difficult to achieve [1, 2] due to their flexible and multipurpose utilization (different operating configurations and use for different productions). To guarantee batchto-batch reproducibility and improve yield and selectivity, automation of batch reactors must be largely increased. Due to the complexity of the reactions mixture and the difficulties to perform on-line composition a measurement, control of batch and fed-batch reactors, is essentially a problem of temperature control [3, 4]. Batch and fed-batch reactors require good temperature control due to the existence of heat-sensitive chemical reactants and/or products and also to the dependency of reaction rate on the temperature. To carry out chemical reactions in this type of reactors, frequently an operating mode consisting of the different phases is used:

- (i) a heating phase of the reaction mixture until the desired reaction temperature,
- (ii) A reaction phase during which the temperature is maintained constant,
- (iii) A cooling phase to avoid by-products formation [5-7].

Any controller was used to controlling the reactor must be able to take into account these different stages [8–11]. The temperature of the reactor content is controlled by the heat exchange with a fluid flowing inside the jacket surrounding the reactor. It is complicated by the operating mode and the numerous fluids to be managed. The control performances are then mainly dependent on the heating-cooling system associated with the reactor [12]. Many studies have been performed on control problems and strategies in such a type of reactors [13, 14].

Many configurations of heating/cooling systems are cited in the literature [13]. Two main types of heating/cooling systems are commonly used in industry: the alternative system or multifluid and mono-fluid system [15, 16]. With the multifluid system, the utility fluids flow alternatively in the jacket depending on the required control variable. The utility fluids are available to a given temperature (plant utilities). This system represents the most largely used system in industry due to the relative ease of design and low cost (direct use of plant utilities). Therefore, the control task of this type of process is rather difficult and can be divided in two parts: firstly, the choice of the right fluid and, secondly, the appropriate action on the flow-rate of this utility fluid in order to satisfactorily track the desired temperature profile. Thus, to go from heating to cooling, a change of fluid is required which results in a discontinuity in the operation.

An alternative configuration is the mono-fluid system which tends to replace the multifluid system in recently built workshops. This system uses only one fluid, the temperature of which can be modified to achieve the desired reactor temperature by an intermediate thermal loop, which may include heat exchangers, power heaters, and so forth; nevertheless, the dynamics of this external thermal loop can be penalizing, particularly in the case of urgent need of a rapid cooling or heating [17]. This technique has been studied earlier [15, 18].

The principle of functioning consists in choosing the apparatus or the fluid to be injected into the thermal loop and then to determine the manipulated variable, which will make it possible to follow a given profile of temperature. This variable can be an electrical power or a flow-rate. This choice is carried out by a program of supervision. Many authors have studied both heating/cooling systems and the supervision. Among the authors [13] presented experimental and simulation studies for temperature control of industrial batch reactors (16, 65, and 160l) equipped with a multifluid heating/cooling systems. They used adaptive GPC with double models references and the supervision strategy based one the limits thermal flux analysis. A new tuning approach of the GPC algorithm has been proposed by [19] in both adaptive and non-adaptive configurations for a fed-batch penicillin process using the complete factorial design method. Another approach for the management of the fluids was developed by [20]. This approach is based on the principle of the supervision by prevision of limit trajectories of temperature. The tool of supervision calculates two criteria every period of sampling, with regard to the distance enter the set-point temperature of the reaction mixture and the evolution which would present the system with a maximum and minimum thermal flux of each fluid.

An effective approach to the control of reactor and similar processes utilizes various methods of the nonlinear control (NC). Several modifications of the NC theory are described in, for example, [21, 22]. Especially, a large class of the NC methods exploits linearization of nonlinear plants, for example, [23], an application of PID controllers, for



FIGURE 1: Schematic of the pilot-plant.

example, [24], or factorization of nonlinear models of the plants on linear and nonlinear parts, for example, [25–27].

This paper deals with a new methodology of supervision and control for the thermal behavior of reactor equipped with a mono-fluid heating/cooling system.

A master controller calculates the thermal flux (can be exchanged between the reaction and the jacket) necessary to flow the required reactor temperature profile. On the other hand, the maximum and minimum thermal capacities of each thermal fluid are determined and used to choose the "right" fluid with the priority to the fluid present in the jacket. The required thermal flux calculated by the master controller is compared to the limit capacities of the present fluid. The master controller is a Predictive Functional Control (PFC). Chosen for its capability to maintain the flexible character of reactor. After a description of the reactor (pilot plant). In the third part, methodology for monitoring and the control of batch reactors are described. Then a brief description of the procedure of regulation (PFC). One gives the strategy of supervision in the fourth part. The last part is devoted to the validation of the system of supervision based on the strategy of management of the thermal devices by the analysis of heat flux. Obtained results, for the thermal behavior of batch reactor in simulation following profiles of typical temperatures (heating-maintenance-cooling-maintenance).

#### 2. Process Description

A schematic diagram of the pilot plant is depicted in Figure 1.

The experimental device consists of a 1 L jacketed glass reactor, equipped with a mono-fluid heating/cooling system. The mono-fluid used in this work is a mixture of ethylene glycol and water, in a ratio of 50% in weight, with a flow rate of 1000 L h<sup>-1</sup> and at a temperature which varies between -35 and  $110^{\circ}$ C. the mono-fluid flow-rate is measured by means of two flow-meters, one installed on the main thermal loop (flow-meter 1) and the other one on the secondary thermal loop (flow-meter 2). The heating/cooling system

uses an electrical resistance of 2000 W and two plate heatexchangers (PHE). One PHE uses cold water as a utility fluid at a temperature around 15°C and a maximum flow rate of  $1500 L h^{-1}$  while the other one uses a mixture of ethylene glycol and water, in a ratio of 50% in weight, at a temperature around of -10°C and a maximum flow of  $1500 \text{ L} \text{ h}^{-1}$ . Flow rates of the utility fluids are also measured. Three on-off valves allow the mono-fluid to be heated or cooled. Two other on-off valves are used to manipulate the utility fluids. A three-way air-to-open valve ensures the division of the mono-fluid in two parts during the cooling phases. A gearing pump ensures the circulation of the monofluid in the thermal loop at maximum flow rate of 1500 L  $h^{-1}$ . The reactor has the following physical specifications: an internal diameter of 82 mm, a wall thickness of 9 mm, an external jacket diameter of 125 mm, a jacket wall thickness of 5 mm, a maximal reactant mixture-reactor heat transfer area of  $0.039 \text{ m}^2$  and a jacket volume of 0.15 L. A propeller rotated at 260 rpm. The reactor is operated in batch and fed-batch modes. A piston pump allows the variation of the liquid reactant flow rate from 0 to  $336 \text{ cm}^3 \text{ h}^{-1}$ .

All the temperatures are measured at each sampling period using PT100 platinum resistance sensors with a precision of  $\pm 0.1^{\circ}$ C. The feed temperature of inlet reactant is measured by a thermocouple. A computer with analogto-digital (A/D) and digital-to-analog (D/A) converters is employed for data acquisition. The supervision and control algorithms programs are written in Fortran 4 and are implemented on a PC in order to accomplish the different temperature control tasks.

## 3. Methodology for Monitoring of Batch Reactor

A strategy integrating the followup and control was developed by [13, 28, 29]. For a batch reactor of 16 L equipped with a heating/cooling system grouping together at once of multifluid and the mono-fluid. To realize the thermal behavior of this process, it also used generalized adaptive predictive control with double model reference (GPCMR).

For the study of the behavior of the process, the structure of regulation in cascade using the technique of predictive functional control (PFC) is application year. Two control levels "1" and "0" are considered. Two controllers are used in the control level "1." The first one in charge of supervision (PFCM), it computes the required thermal flux to be exchanged between the mono-fluid flowing inside the jacket and the reaction mixture. The second one (PFC1) is devoted to calculate the set-point temperature  $(T_{icons})$  which will be tracked by the inlet jacket temperature. In the control level "0," because the algorithm of the PFC is an algorithm SISO (single input, single output), three slave controllers are used to control the mono-fluid temperature. One placed on the electrical resistance which computes the electrical power value and the other two on the two plant heat exchangers to compute the mono-fluid flow rate fraction dispatched to one of them.



FIGURE 2: Schematic of the plant block en cascade control.

The plan block for cascade control of this process is given in Figure 2.

The model has been established using the following basic assumptions:

For the reactor.

- (i) Specific heat and density of pure components are constant in the considered range of temperature, the heats of mixing are neglected.
- (ii) The reactions are carried out in a pseudohomogeneous liquid phase.
- (iii) If the reactions would be put into play, the heats of reactions are taken into account.
- (iv) The reactor is perfectly mixed with homogeneous temperature and concentrations in the reaction mixture.
- (v) Feeding of the reactive is performed without volume concentration.
- (vi) The kinetic laws of the chemical reactions involved are assumed to be such that the reaction rate constant follows the Arrhenius law and the reaction rate is a function of the reactant concentrations.

*3.1. Electrical Resistance.* To model the electrical resistance, we considered spaced out annular as a block stirred, in which the monofluid exchanges some heat with the wall of the stem and receives a heat flux resulting from the electric resistance.

*3.1.1. Heat Exchangers.* Heat and cold currents are always parallel between the input and output device.

No the phase change and the physical properties of both fluids and plate remain constant in the temperature range used.

Heat loss with the external environment is considered negligible.

The flow of the two fluids is of piston type. For each fluid, the speed is the same on any plane normal to the direction of the currents, so there is only temperature gradient in the direction parallel to the currents.

The total exchange surface is the sum of the exchange surfaces of all plates.

The writing the thermal balances, reflecting the exchange between the reaction mixture and the jacket of the reactor, led us to use the thermal flux as a control variable intermediary. This variable can then simultaneously solve the problem of supervision and control. Moreover, this control strategy is applicable to any thermal system.

*3.1.2. Thermal Behavior of the Reactor.* The reactor can be described by the following thermal balances.

Thermal balance on the reaction mixture:

$$\rho_r C p_r V_r \frac{dT_r}{dt} = U A_{r, \text{pr}} (T_{\text{sde}} - T_r) + F_c \rho_c C p_c (T_c - T_r) - \mathcal{Q}_r.$$
(1)

Initial conditions: the physico-chemical properties ( $\rho$ , Cp, V, U, F, Q,  $T_c$ ) are data (constants).

 $T_{\rm sde}$  calculated by (11).

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Thermal balance on the mono-fluid flowing inside the jacket:

$$\rho_{\rm fc} C p_{\rm fc} V_{\rm de} \frac{dT_{\rm sde}}{dt} = U A_{r,\rm pr} (T_r - T_{\rm sde}) + F_{\rm fc} \rho_{\rm fc} C p_{\rm fc}$$

$$\times (T_{\rm ede} - T_{\rm sde}).$$
(2)

Initial conditions:  $\rho_{\rm fc}$ ,  $F_c$ ,  $Cp_{\rm fc}$ ,  $V_{\rm de}$ ,  $UA_{r,\rm pr}$ ,  $F_{\rm fc}$  are data.  $T_{\rm ede}$  is the temperature of the utility used by the cooling heat exchanger:  $T_e = T_{\rm fc0}$  (cold water),  $T_e = T_{\rm fc0}$  (glycol water).

Tow controllers are used in the main controller loop, the first one called PFCM in charge of supervision; and the second one called PFC1 devoted to compute the jacket setpoint temperature used by the slave controllers.

The internal model used by the PFCM controller was derived from (1) and it is given by the following continuous system transfer function equation using the Laplace transform:

$$T_{r}(p) = \left[\frac{1}{UA_{r,pr}}\right] \frac{1}{\tau_{r}p} \left(U_{q}(p) + \mathcal{Q}_{ech}(p)\right)$$

$$T_{r}(p) = \frac{K}{p} \left(U_{q}(p) + \mathcal{Q}_{ech}(p)\right),$$
(3)

where  $\tau_r = \rho_r C p_r V_r / U A_{r,pr}$  time constant of the reactor,  $U_q = U A_{r,pr} (T_{sde} - T_r)$  the thermal flux exchanged between reaction mixture and the mono-fluid present inside the jacket,  $Q_{ech} = F_c \rho_c C p_c (T_c - T_r) - Q_r$  the disturbance caused by feed reactants and the heat released by the chemical reaction,  $K = 1/\tau_r U A_{r,pr}$  is the steady-state reactor gain (PFCM controller).

The following model was proposed to construct the PFC1 controller:

$$T_r(p) = \frac{K_r}{1 + \tau_r p} T_{ede}(p) + \frac{K_c}{1 + \tau_r p} T_c(p) + \frac{K_{Qr}}{1 + \tau_r p} Q_r(p).$$
(4)

where  $K_r$  is the steady-state reactor gain (PFC1 controller),  $K_c$  the steady-state liquid reactant feed gain,  $K_{Qr}$  the steady-state heat released gain.

#### 4. Supervision Strategy

The objective of the thermal behavior of the batch or fedbatch reactors equipped with a mono-fluid heating/cooling system is to be simultaneously able to determine the element of the thermal loop which is going to modify the temperature of the mono-fluid, as well as commands it to apply to the chosen actuator, to reach the objective of the regulation. The protocol of the thermal conduct is based on the following concept.

The regulator calculates the control variable which is interpreted as a thermal flux. This last one is then compared with thermal flux limits, calculated on-line for the various devices to choose the adequate element of the thermal loop. Once this choice realized, the manipulated variable is calculated according to the chosen device.

#### 4.1. Limit Thermal Capacities

4.1.1. Electrical Resistance. This element of the thermal loop is used to heat the mono-fluid that can receive a maximum electric power  $P_{elec}$  (max).

This maximum power will be considered as the maximum flux that can be exchange the mono-fluid with the reaction mixture through the jacket.

The evolution of the outlet temperature of the electrical resistance is given by the following thermal balance:

$$\left(\frac{V_{\rm ch}}{F_{\rm fc}}\right) \frac{d\left(T_{\rm ch} - T_{\rm ch}^E\right)}{dt} = \left(T_{\rm ch} - T_{\rm ch}^E\right) + \frac{P_{\rm elec}(\max)}{\rho_{\rm ch}Cp_{\rm ch}V_{\rm ch}}U_p,$$
$$0 \le U_p \le 1.$$
(5)

We distinguish two limits maximum thermal flux  $(Q_{\text{max ch}})$ and minimum  $(Q_{\text{min ch}})$ , such as

$$Q_{\text{max ch}} = P_{\text{elec}}(\text{max})$$

$$Q_{\text{min ch}} = 0.0.$$
(6)

4.1.2. Plate Heat Exchangers. It uses two thermal balances to calculate the thermal flux limit corresponding to these two heat exchangers. The first concerns the mono-fluid during its passage through the jacket and the other is the interchange between the reaction mixture and mono-fluid present in the jacket.

These balance sheets are translated by following equations:

$$Q_1 = F_{\rm fc} \times \rho_{\rm fc} \times C p_{\rm fc} (T_e - T_s), \tag{7}$$

$$Q_{2} = U \times A_{r, \text{pr}} \left( \frac{(T_{e} - T_{r}) + (T_{s} - T_{r})}{2} \right),$$
(8)

$$\frac{1}{U} = \left[\frac{1}{U_{r,\text{pr}}} + \frac{1}{U_{\text{pr,fc}}} + \frac{A_{r,\text{pr}}}{A_{\text{pr,fc}}}\right].$$
(9)

The whole methodology, for the computation of the control variable, relies on the assumption that both thermal fluxes are equal:

$$Q_1 = Q_2. \tag{10}$$



FIGURE 3: Evolution of the thermal flux capacities for the different fluids.

From (7), (8) and (10), the outlet temperature of the jacket is calculated by the following relation:

$$T_{s} = \frac{\left(F_{\rm fc} \times \rho_{\rm fc} \times Cp_{\rm fc} - U \times A_{r,{\rm pr}}/2\right) \times T_{e} + U \times A_{r,{\rm pr}} \times T_{r}}{F_{\rm fc} \times \rho_{\rm fc} \times Cp_{\rm fc} + U \times A_{r,{\rm pr}}/2}.$$
(11)

The flow rate of the mono-fluid being constant, during the cooling the minimal temperature which can be reached the entry of the jacket, is the one of the temperature of the utility of cooling used by the heat exchanger. That makes it possible to write:

 $T_e = T_{fc0}$  (Cold water): in the case of the heat exchanger using cold water.

 $T_e = T_{fc0}$  (Glycol water): in the case of the heat exchanger using the glycol water.

To calculate these minimal thermal flux  $Q_{\min ef}$  and  $Q_{\min eg}$ , corresponds to the use of heat exchangers with cold water and with glycol water respectively, we will use the equations (7) or (8) by taking as external temperature of  $T_s$  that calculated by the equation (11).

We consider that the maximum thermal flux, corresponding to the use of heat exchangers with cold water and with glycol water respectively, is zero.

When a thermal equilibrium at the level of the double envelope,  $(T_e = T_s)$  will occur:

$$Q_{\text{max ef}} = 0,$$

$$Q_{\text{max eg}} = 0.$$
(12)

4.2. Supervision Algorithm. Figure 3 gives an approximate global representation of the evolution of the thermal flux capacities of the different fluids as a function of the reactor temperature; the minimum and maximum capacities correspond to the border of the zones. Three zones are distinguished.

Zone 1: use the electrical resistance.

Zones 2: use of the heat exchanger with cold water. Zones 3: use of the heat exchanger with glycol water.

When the thermal flux takes a positive value, it corresponds to a demand for heating and only the electrical resistance is concerned (phase = 1). A negative value means a request of cold; in this case one of both heat exchangers will be used according to the value of the thermal flux. So, a value in the range ( $Q_{\min ef}$ ,  $Q_{\max ef}$ ), means a request of cooling by cold water, then only the heat exchanger in cold water is concerned (phase = 2) a value in the range ( $Q_{\min eg}$ ,  $Q_{\min ef}$ ), means a request of cooling by the glycol water and only the heat exchanger for glycol water is concerned, (phase = 3). A flow chart of the overall procedure is given in Figure 4.

#### 5. Results and Discussion

In this paper, we present the simulation results obtained for the temperature control of an exothermic chemical reaction of acid-base neutralization between the hydrochloric acid (HCl) and the sodium hydroxide (NaOH).

The set-point temperature profile is composed by first stage: heating from 20 to 40°C during 1000 s; second stage: constant temperature at 40°C during 1500 s; third stage: cooling from 40 to15°C during 1200 s and fourth stage: maintain at 15°C during 500 s.

However, the temperature profile is composed by an increase ramp-maintain and decrease ramp-maintain. In order to eliminate discontinuities resulting from change of stage, the set-point profile was filtered by a procedure called "docking procedure" [8, 17, 30]. The results are presented in Figure (5–7).

Figure 5 we can notice that the adjusted set-point temperature ( $T_{cons}$ ) is correctly followed by the reaction temperature ( $T_r$ ) and ( $T_{cdoc}$ ) during almost all the profile of temperature. The only exception, concerns the beginning of the phase of maintenance and the phase of cooling a slight difference appears then of the change of device. This slight difference is also translated by the evolution of the thermal flux ( $U_q$ ) (Figure 7).

Figure 6 shows the evolution of the manipulated variable  $(\beta)$  which corresponds or in the fraction of the power of heating power calculated by the regulator during use of the electrical resistance or in the fraction of the flow-rate of the mono-fluid calculated during the use of the heat exchanger with cold water either the heat exchanger with glycol water. In the figure, this variable corresponds to the fraction of the heating power during a much of the profile.

Figure 7 shows a regular evolution of the required thermal flux. This variable takes a positive value in time equal has zero to 2400 s ( $U_q > Q_{\min ch}$ ) allowing the use of the electrical resistance and when it becomes negative ( $Q_{\min ef} < U_q < Q_{\max ef}$ ) in time equal 2430 s to 2610 s it allows the use of PHE which uses the cold water and at times equals 2790 s to 3810 the use of PHE with glycol water, then to 3840 s it takes a positive value. We can notice that  $U_q$  plays a role of real supervisor because it permits the change of apparatus only when there are an urgent heating or an urgent cooling



FIGURE 4: Flow chart of the supervisory and control in the case of the electrical resistance.



FIGURE 5: Evolution of temperature ( $T_{cons}$ ), the adjusted set-point ( $T_{cdoc}$ ), and reaction mixture ( $T_r$ ), K = 0.5,  $K_r = 1$ .

without provoking deterioration in the followup of the setpoint profile.

Another simulation has been performed for a different set-point profile, with the hydrochloric acid solution was introduced to 1800 s. The simulation consists in a four-step temperature set-point profile.

1st phase: heating from 20 to 30°C during 1000 s.

2nd phase: constant temperature set-point of 30°C during 5000 s.

3rd phase: cooling from 30°C to 20°C during 1000 s.



FIGURE 6: Evolution of the manipulated variable ( $\beta$ ), K = 0.5,  $K_r = 1$ .

4th phase: constant temperature set-point at  $20^{\circ}$ C during 500 s.

Results are given in Figures (8–10).

Figure 8 show that at the beginning of the feeding the reaction mixture temperature  $(T_r)$  exceeds the setpoint temperature  $(T_{cons})$  and  $(T_{cdoc})$ . The regulation system reacts always by commuting of the electrical resistance as indicated on Figure 9, and also represents this disturbance translated by the oscillations of the manipulated variable  $(\beta)$ (Figure 10). At the end of feeding, we observe one under overtaking of 1°C approximately, which are due to the fact that the temperature of the mono-fluid is close of 30°C and the system late to return on the landing.



FIGURE 7: Evolution of thermal flux and limits thermal flux, K = 0.5,  $K_r = 1$ .



FIGURE 8: Evolution of temperature ( $T_{cons}$ ), the adjusted set-point ( $T_{cdoc}$ ), and reaction mixture ( $T_r$ ), K = 1,  $K_r = 0.5$ .

Figure 9 we can observe that the thermal flux in time 5940 s is negative in the range of use of the PHE with cold water and 5970 s until 6000 s the use of the PHE with glycol water then we observe afterward the quality of thermal behavior becomes correct again.

To demonstrate, once again, the performance of the strategy of supervision another simulation has been performed for set-point profile of an exothermic reaction of mononitration with a desired constant temperature of 30°C for various conditions.

1st phase: heating from 20 to 30°C during 1000 s.

2nd phase: constant temperature set-point between 1000 s and 14800 s with feeding.

3rd phase: cooling from 30°C to 20°C during 1000 s.

4th phase: constant temperature set-point at  $20^{\circ}$ C during 500 s



FIGURE 9: Evolution of thermal flux and limits thermal flux, K = 1,  $K_r = 0.5$ .



FIGURE 10: Evolution of the manipulated variable ( $\beta$ ), K = 1,  $K_r = 0.5$ .

Results are given in Figures (11, 12, and 13).

Figures (11–13) show at the time of the introduction of feeding, which is then accompanied by a thermal bad behavior characterized by the oscillations of the thermal flux, the manipulated variable ( $\beta$ ), and the temperature of the reaction mixture, and that for the duration of feeding until the end of the feeding. These oscillations are due to the fact that we did not take into account the release of heat in the model of supervision what generated afterward problems of behavior which are not easy to master.

In addition, if you want the results justified physically by noting that for Figures 5, 6 and 7 obtained for K = 0.5 and  $K_r = 1$ , the control quality is very good throughout the setpoint profile.

Figures 8 to 10 obtained for K = 1 and Kr = 0.5, show that one on the other hand has a little unstable behavior for the values K = 0.5 and KR = 0.5 one obtains a very unstable behavior as indicated on Figures 11 to 13.

Analysis of these results shows a value of 1 for the static gain  $K_r$  is essential for the master controller is effective while



FIGURE 11: Evolution of thermal flux and limits thermal flux, K = 0.5,  $K_r = 0.5$ .



FIGURE 12: Evolution of the manipulated variable ( $\beta$ ), K = 0.5,  $K_r = 0.5$ .

for the regulator responsible for monitoring a value of K in the range from 0.5 to 1 works well.

Note that the controller is the most critical PFC1, it acts as a master controller while PFCM is used for supervision, and its role becomes crucial only in the stages of change of device.

## 6. Conclusion

A new methodology of control and supervision has been developed. It is based on choosing as manipulated variable the thermal flux to be exchanged between the reaction mixture and the jacket. This required flux calculated by the master controller is then used in model based supervisory structure which, according to the limit capacities of the different fluid configurations. In this paper, this methodology has been applied to a mono-fluid heating/cooling system.

The application of such a methodology to pilot-plant batch reactor has been represented. It turned out that at least good basic modeling of the process in necessary. Thus the choice of internal model is crucial importance for (PFC),



FIGURE 13: Evolution of temperature ( $T_{cons}$ ), the adjusted set-point ( $T_{cdoc}$ ) and reaction mixture ( $T_r$ ), K = 0.5,  $K_r = 0.5$ .

since the capacity of prediction constitutes the base of all the specifications of performance. However, it is necessary to know the parameters related to the reaction with a certain degree of accuracy. Even if the batch reactor must remain polyvalent, the reactions were generally subject to a certain number of studies. Otherwise, simulation studies have shown when the heat released by the chemical reaction was considered, the control system permits a better tracking of the set-point temperature profile. This strategy is not limited to a mono-fluid heating/cooling system presented in this paper, but may be extended to any system whatever the number of fluids. Therefore the supervision technique can be considered as an appropriate solution for the temperature control of batch reactors, and the developed control strategy can be implemented to control industrials batch reactors.

## Nomenclature

- $A_{r,pr}$ : Heat transfer area between the reaction mixture and the reactor wall, m<sup>2</sup>
- $A_{\rm pr,fc}$ : Heat transfer area between the reactor wall and the mono-fluid, m<sup>2</sup>
- $Cp_{fc}$ : Specific heat of the mono-fluid, KJ/Kg·K
- $Cp_{ch}$ : Specific heat of the mono-fluid flowing inside the electrical resistance, KJ/Kg·K
- $Cp_r$ : Specific heat of reaction mixture, KJ/Kg·K
- $Cp_c$ : Specific heat of liquid reactant feed, KJ/Kg·K
- $F_c$ : Liquid reactant feed flow rate, m<sup>3</sup>/s
- $F_{\rm fc}$ : Mono-fluid flow rate through the double-envelope,  $m^3 \cdot s^{-1}$
- $F_{\rm fc}$ : Utility fluid flow rate, m<sup>3</sup>/s
- *K*: Steady-state reactor gain (PFCM controller), K/KJ
- *K<sub>r</sub>*: Steady-state reactor gain (PFC1 controller)
- *K<sub>c</sub>*: Steady-state liquid reactant feed gain
- $K_{Qr}$ : Steady-state heat released gain, s·K/KJ

 $P_{\text{elec (max)}}$ : Maximum electrical power value, KJ/s

cice (max)	1 , , ,
$Q_{\min ef}$ :	Minimal thermal flux of the cold water, KJ/s
Q <sub>max ef</sub> :	Maximal thermal flux of the cold water, KJ/s
$Q_{\min eg}$ :	Minimal thermal flux of the ethylene
	glycol/water, KJ/s
Qmax eg:	Maximal thermal flux of the ethylene
cinar eg	glycol/water, KJ/s
<i>O</i> <sub>min ch</sub> :	Minimal thermal flux of the electrical resistance,
<b>C</b>	KJ/s
Omax ch:	Maximal thermal flux of the electrical
	resistance, KI/s
$Q_r$ :	Heat released by the chemical reaction, KJ/s
$T_e$ :	Inlet jacket temperature, K
$T_c$ :	Liquid reactant feed temperature, K
$T_{\rm ch}$ :	Mono-fluid temperature at the outlet of the
	electrical resistance, K
$T_{\rm ch}^E$ :	Mono-fluid temperature at the inlet of the
	electrical resistance, K
$T_{cdoc}$ :	Docking set-point temperature, K
$T_{\text{cons}}$ :	Set-point temperature, K
$T_r$ :	Reaction mixture temperature, K
$T_s$ :	Outlet jacket temperature, K
$T_{sde}$ :	Outlet monofluid temperature, K
U:	Heat transfer coefficient between the
	mono-fluid and the reaction mixture, KJ/m <sup>2</sup> · s
	K
$U_{\rm pr,fc}$ :	Heat transfer coefficient between the reactor
	wall and the mono-fluid, KJ/m <sup>2</sup> · s K
$U_p$ :	Fraction of the power of heated $0 \le U_p \le 1$
$V_r$ :	Volume occupied by the reaction mixture inside
	the reactor, m <sup>3</sup>

- Greek Letters
- $\rho_r$ : Density of reaction mixture, Kg/m<sup>3</sup>
- $\rho_c$ : Density of liquid reactant feed, Kg/m<sup>3</sup>
- $\rho_{ch}$ : Density of mono-fluid inside the electrical resistance, Kg/m<sup>3</sup>
- $\rho_{\rm fc}$ : Density of mono-fluid out the jacket, Kg/m<sup>3</sup>.

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