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A new strategy for temperature control of batch reactors: experimental application

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Abstract

In this paper, a new strategy for temperature control of multipurpose batch reactors using a cascaded model based control is presented. This strategy is based on the use of the thermal flux as the manipulated variable. At each sampling time, the master controller computes the thermal flux to be exchanged between the reactor content and the thermal fluid flowing inside the jacket. This information is then used to determine the right fluid and to evaluate the opening value of the control valve. For this purpose a physical modelling of the thermal system has been developed. Finally, the control valve opening degree is computed and applied to the plant. © 1999 Published by Elsevier Science S.A. All rights reserved.

Keywords: Process control; Batch reactor; Fine chemistry; Model based control; Adaptive predictive control

1. Introduction

In fine chemical or pharmaceutical industry, the batch or fed-batch reactor functions as the heart of the process transformation. Due to the complexity of the reaction mixture and the difficulty to perform on-line composition measurements, control of batch reactors is essentially a problem of temperature control [6].

Temperature control of batch reactor is a problem which is difficult to overcome [7]. The difficulties arise in part from the discontinuous nature of the operating modes and in part from the various uses of these reactors. The regulator must work in the face of drastic changes in set-points and also be adaptable to the different modes of operation. To carry out chemical reactions in this type of reactors, frequently an operating mode consisting of different phases is used:

- A heating phase which allows preheating of the reaction mixture up to the desired temperature.
- A reaction phase during which the temperature is maintained constant.
- A cooling phase to avoid by-products formation.

The temperature of the reactor content is controlled by 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 [1]. A lot of studies have been performed on control problems and strategies in such a type of reactors. Chylla and Randall Hasse [3] and Juba and Hamer [7] give a good overview on the challenges in batch reactor control and suggest several control strategies.

Many configurations of heating–cooling systems are cited in literature. The two common types of heating–cooling systems are the alternative heating–cooling system (90% of industrial applications) and the mono-fluid system.

The multi-fluid system is commonly used in the industry. Either a cooling (cold water, brine) or a heating fluid (steam, hot water) is delivered to the jacket according to the need. In this area besides the work undertaken in our laboratory [8,10] very few papers have been published [3,9]. Control of this arrangement is quite difficult since the choice of the fluid circulating and its flowrate have to be decided in order to track satisfactorily the desired temperature profile. Thus, to go from heating to cooling, a changeover of fluid (with intermediate air-purge of the jacket) is required which results in a discontinuity in the operation. Hence this arrangement permits to work in a wide range of temperatures.

The mono-fluid system uses a single-fluid the temperature of which can be modified to achieve the desired reactor temperature by an intermediate thermal loop which may

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include heat exchangers, power heaters, etc.... Nevertheless, the dynamics of this external thermal loop can be penalising, especially in the case of urgent need of a rapid cooling or heating. This technique has been investigated earlier [8,9]. Control of this system is often done by cascading two control loops.

Thermal control of flexible and multipurpose batch reactors is difficult to achieve with conventional PID controllers. In the fine chemical and pharmaceutical industry, many different reactions with variable operating conditions are carried out in the same reactor and the parameters of the PID controller require frequent retuning to adjust them to these different operating conditions. In previous studies [8,10], it has been shown that adaptive model predictive control can answer to this flexible character.

Up to now, the choice of the fluid has generally been carried out by an external structure based on alarm levels. Nevertheless, the definition of this structure is difficult and never satisfying. The use of the thermal flux as intermediate control variable allows to solve this problem. It is possible to compute on-line the range of thermal flux available for each fluid. Then, by comparison of the required thermal flux with the up and low limits of each fluid, the fluid to be used could be chosen.

This paper deals with a new strategy of temperature control of batch reactors. Its principle is based on considering as manipulative variable the thermal flux delivered/removed to the reaction mixture to track the desired temperature profile. This thermal flux is computed by the master controller and then used in a cascade-like structure to firstly determine the right configuration of the heating–cooling system which can deliver this flux (the heating/cooling element in the case of the mono-fluid system or the fluid in the case of the multi-fluid system) and secondly to compute the actual control action.

Of course, this control strategy could be applied to any type of heating–cooling systems (multi-fluid system, mono-fluid system,...). But to improve controllability of batch reactors we have also designed a different heating–cooling system which takes advantage of the superiorities of the previous systems. The idea is to take opportunity of the advantages of both systems: multi-fluid with large heating (cooling) capabilities of steam (glycol water) when rapid heating (cooling) is needed and mono-fluid for normal operating conditions as it is better to use a single-fluid circulating at a sufficiently rapid flowrate to get a good heat transfer coefficient. This system presents the advantages of a multi-fluid thermal system (possibility to use utility fluids directly available on a plant) and those of mono-fluid thermal system (characterized by high dynamic performance and continuity of thermal control). During a classical operation it is necessary to change from a configuration to another. Instead of a classical alarm-based method the supervisory strategy is based on the thermal flux computation as described previously. The master controller is an adaptive predictive control algorithm (''generalized predictive control with double model reference'') chosen for its capability to maintain the flexible character of the reactor. Once the configuration has been chosen, the control action corresponding in delivering the required thermal flux is then determined by using a physical modelling of the thermal system.

2. Process description

To overcome the strong discontinuities due to the change-over from hot to cold utilities as done traditionally with multi-fluid systems, we propose to use an intermediate system obtained by mixing cold water and steam. This new heating–cooling system is an hybrid configuration [2] which integrates the advantages of both the mono-fluid and multi-fluid systems:

- during normal conditions, a single-fluid (intermediate fluid) circulates at a fixed flowrate (high enough to ensure good heat transfer coefficients) and its temperature is modified according to the required thermal flux computed by the controller by acting on the quantity of injected steam (or cold water in the case of fluid recycling),
- for extreme temperature conditions steam or glycol/water are directly used (as in the case of the multi-fluid system); the utility flowrate is changed according to the required thermal flux.

It may be noted that the advantages of this strategy, based on supervisory control according to thermal flux limits, not only makes the heat exchange capacity vary continuously but enables an adequate change of system configuration, from multi-fluid to mono-fluid configuration.

A pilot plant consisting of a stirred batch reactor of 16 l is used for this work. The reactor is a glass-lined batch reactor of maximum operating volume of 12 l. Its internal diameter is 0.30 m, its external diameter is 0.40 m, the height of the jacket is 0.30 m. It is supplied with a mixer of 0.21 m diameter which rotates at approximately 360 rpm, the jacket volume is 10 l. Air is used for emptying the jacket when a change of fluid is operated. Three utility fluids are available at a given temperature for control: 6 bar steam, cold water at about 15°C (pressure 2 bar), mixture of monopropylene glycol and water (50/50 weight) at a temperature of -10°C. The intermediate fluid is obtained by direct mixing of cold water and steam, its temperature varies as a function of the steam-valve opening and the maximum attainable temperature is limited at about 70°C.

The pilot reactor (Fig. 1) is surrounded by a pipe-net for each thermal fluid delivery which is fitted out with the instruments necessary for data acquisitions and control. These instruments include sensors of temperature, pressure and flowrate for every fluid. Six temperature sensors (Pt 100) are used to measure the following temperatures: jacket inlet temperature, jacket outlet temperature, mixer outlet

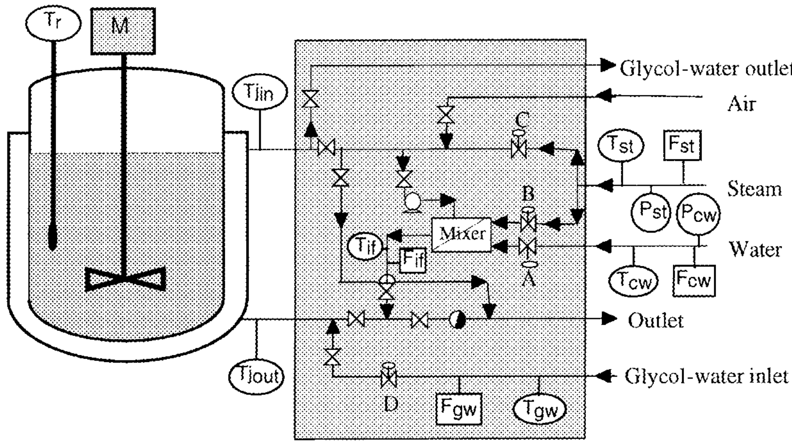


Fig. 1. Experimental pilot plant reactor.

temperature, cold water inlet temperature, steam temperature, reactor temperature. Four sensors are used to measure the following values: glycol/water flowrate, cold water flowrate, intermediate fluid flowrate, steam flowrate. The actuators on the pilot plant include two types of valves: on-off valves and proportional valves. Four proportional valves are implemented which allow to control the flowrates of thermal fluids available on the pilot plant as follows:

- cold water flowrate (A),
- steam flowrate (C),
- steam to be mixed with cold water flowrate (B),
- glycol/water flowrate (D).

Each valve is connected to an electropneumatic converter. Twelve on-off valves are used on the different thermal fluids net and are activated when a changeover of configuration is required. Two possibilities can be studied: without recycling of the intermediate fluid and with recycling by means of a pump. This later one allows energy saving by using exact quantities of steam or cold water necessary to get the desired temperature at the jacket inlet.

3. A new methodology for supervision and control of batch reactors

A new strategy integrating supervisory and control together is proposed. A master controller computes the thermal flux to be exchanged between the reactant mixture and the jacket, necessary to achieve the required reactor temperature profile. On the other hand, the maximal and minimal thermal capacities of each thermal fluid (steam, intermediate fluid, glycol/water) are then determined and used to choose the "right" fluid according to these thermal limit capacities with a priority to the fluid present in the jacket. These limit capacities of heating and cooling of each thermal fluid are calculated on-line by a procedure involving the reaction mixture temperature, the jacket inlet and outlet temperatures, the physical properties of the fluids and the value of the manipulated variable delivered by the controller (see Section 3.4).

3.1. Master control loop

In this work, an adaptive and predictive controller (the "Generalized Predictive Controller with double Model Reference": GPCMR, ([4,8,10])) is used in the master loop to compute the thermal flux to be exchanged between the reaction mixture and the jacket in order to track the desired reactor temperature profile. Details of this algorithm and its use for temperature control of batch reactor can be found in ([8]). This adaptive controller is based on a linear input–output representation of the process.

An advantage of using the thermal flux as manipulated variable is that the process can be modelled as a linear system which was not the case with the classical strategy consisting in acting on the flow of the thermal fluid, leading to very strong non-linearities ([8]). Neglecting the external thermal losses, and in the case without heat released by a reaction, the thermal evolution of the reactor temperature is described by

$$\frac{\mathrm{d}}{\mathrm{d}t}(mC_p\,(T_\mathrm{r} - T_\mathrm{ref})) = Q. \tag{1}$$

Over a sampling period, it is assumed that the mass (m) and the heat capacity (C_p) are constant. Thus, the following discrete-time model can be derived

$$T_\mathrm{r}(k) - T_\mathrm{r}(k-1) = \frac{\Delta t}{mC_p}Q(k-d), \tag{2}$$

i.e., in a parametric form

$$T_\mathrm{r}(k) + a_1T_\mathrm{r}(k-1) = b_0Q(k-d) + e(k). \tag{3}$$

This model is used as the linear input–output model for the GPCMR controller, where $T_\mathrm{r}(k)$ is the process output, i.e., the reactor temperature, $Q(k)$ is the process input, i.e., the thermal flux exchange between the reactor and the jacket and $e(k)$ is a disturbance, assumed to be a white noise.

To overcome plant/model mismatch (heat capacity variation, reactive feeding, heat losses,...) an on-line estimation of parameters a_1 and b_0 is performed by a classical recursive least-squares, which minimizes the following criterion

$$J = \frac{1}{2}\sum_{k=1}^{N}(T_{\mathrm{mes}}(k) - T_{\mathrm{cal}}(k))^2, \tag{4}$$

where T_{mes} is the measured reactor temperature and T_{cal} is the predicted output based on the estimated parameters.

The parameters are initialized with a priori estimated values of m and C_p. The on-line estimation of the model parameters also allows to compensate errors due to approximations considered for the model development presented in the following (Sections 3.2 and 3.3) and to follow the changes in the dynamics occurring during the different steps: heating, reaction, cooling phases and to correct plant/model mismatches.

3.2. Basic modelling relationships

Both supervisory and control are based on the model of the heat exchanges between the reaction mixture and the jacket.

The thermal flux exchanged by the thermal fluid and the reactor is given by

$$Q_1 = UA\left\{\frac{(T_{\mathrm{j_{in}}} + T_{\mathrm{j_{out}}})}{2} - T_{\mathrm{r}}\right\}, \tag{5}$$

assuming that the jacket wall is uniformly distributed. The thermal flux delivered by the thermal fluid to the reactor depends on the nature of the fluid. For liquids, it is expressed by

$$Q_2 = FC_p(T_{\mathrm{j_{in}}} - T_{\mathrm{j_{out}}}). \tag{6}$$

When steam is injected directly in the jacket, the thermal flux is proportional to the latent heat according to:

$$Q_2 = F_{\mathrm{st}}\mathrm{Lv}. \tag{7}$$

The whole methodology, for the computation of the control variable, relies on the assumption that both thermal fluxes are equal: $Q_1{=}Q_2$.

In the case of liquid fluids, $T_{\mathrm{j_{out}}}$ could be computed from Eqs. (5) and (6), and we get

$$T_{\mathrm{j_{out}}} = \frac{\{T_{\mathrm{j_{in}}}[2FC_p - UA] + 2T_{\mathrm{r}}UA\}}{2FC_p + UA}. \tag{8}$$

The heat transfer coefficient U is computed on-line according to classical correlations ([5]). Heat capacity C_p is expressed as a function of temperature. Nevertheless, very low difference is observed if constant values are assumed.

3.3. Thermal behaviour of the different fluids

Let us now examine the process behaviour according to the fluid delivered to the jacket:

3.3.1. Glycol/water

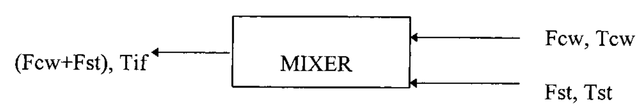
The inlet temperature ($T_{\mathrm{j_{in}}}$) is kept constant and equal to T_{gw} (−15°C in practice). The control action is made on the fluid flowrate F_{gw}.

3.3.2. Intermediate fluid

For this configuration, the flowrate F_{if} is kept constant (500 kg h^{-1} in practice) and the inlet temperature of the fluid ($T_{\mathrm{j_{in}}}$) is modified by the control action.

Two cases have to be considered according to the fact that the intermediate fluid is recycled or not. In the first case, the manipulated variable is either the steam flowrate or the water flowrate depending on whether $T_{\mathrm{j_{in}}}$ must be increased or decreased. In the second case, the water flowrate is kept constant (F_{cw}) and the manipulated variable is the steam flowrate.

3.3.2.1. System without recycling of the intermediate fluid.



The flowrate (F_{if}) of the intermediate fluid is obtained by mixing the cold water stream with a steam flowrate. At the outlet of the mixer, we get

$$F_{\mathrm{if}} = F_{\mathrm{cw}} + F_{\mathrm{st}}. \tag{9}$$

It is assumed that the intermediate fluid has the same properties (C_p) than the cold water (main water). The steam flowrate F_{st} is computed as the following:

$$F_{\mathrm{st}} = \beta\,\mathrm{cvs}\sqrt{P_{\mathrm{st}} - P_{\mathrm{cw}}}, \tag{10}$$

where P_{st} is the steam pressure (6 bar in practice), P_{cw} the pressure of the cold water (main water), β the valve opening degree, cvs is the valve characteristic coefficient. The intermediate fluid temperature (T_{if}) after mixing is given by

$$T_{\mathrm{if}} = T_{\mathrm{cw}} + \frac{F_{\mathrm{st}}\{C_{p_{\mathrm{cw}}}[T_{\mathrm{st}} - T_{\mathrm{cw}}] + \mathrm{Lv}\}}{C_{p_{\mathrm{cw}}}(F_{\mathrm{cw}} + F_{\mathrm{st}})}, \tag{11}$$

where T_{cw} is the inlet temperature of cold water (main water, in practice about 15°C). T_{st} is the temperature of the inlet steam (boiling temperature at P_{st}).

3.3.2.2. System with recycling of the intermediate fluid. A comparison between the calculated inlet temperature, $T_{\mathrm{j_{in}}}$, and the measured outlet jacket temperature $T_{\mathrm{j_{out}}}$ allows to choose the fluid to be injected in the intermediate fluid and to determine the corresponding valve opening degree. Moreover, in practice the flowrate of the intermediate fluid is kept constant (F_{if}) by a trap.

If the temperature of the intermediate fluid has to be increased, steam is injected in the intermediate fluid and the temperature at the outlet of the mixer is given by Eq. (12) where $T_{\mathrm{j_{out}}}$ is measured at the outlet of the jacket.

$$T_{\mathrm{if}} = T_{\mathrm{j_{out}}} + \frac{F_{\mathrm{st}}\{C_{p_{\mathrm{cw}}}[T_{\mathrm{st}} - T_{\mathrm{j_{out}}}] + \mathrm{Lv}\}}{C_{p_{\mathrm{cw}}}(F_{\mathrm{if}} + F_{\mathrm{st}})}. \tag{12}$$

If the temperature must be decreased, the intermediate fluid is then obtained by mixing two water streams, and we get

$$T_{\mathrm{if}} = T_{\mathrm{cw}} + \frac{F_{\mathrm{cw}}[T_{\mathrm{cw}} - T_{\mathrm{j_{out}}}]}{F_{\mathrm{if}} + F_{\mathrm{cw}}}. \quad (13)$$

3.3.3. Steam

The steam flowrate is given by

$$F_{\mathrm{st}} = \beta \,\mathrm{cvs}\, \sqrt{P_{\mathrm{st}} - P_{\mathrm{j}}}, \quad (14)$$

where P_{st} is the steam pressure (6 bar in practice), β the valve opening degree and cvs is the valve characteristic coefficient.

The pressure Pj can be derived from the pressure of air in the jacket (initially at T_0) and the partial pressure of the steam in the jacket according to

$$P_{\mathrm{j}} = \frac{P_{\mathrm{air}} T_{\mathrm{j_{st}}}}{T_0} + P_{\mathrm{j_{st}}}(T_{\mathrm{j_{st}}}). \quad (15)$$

The steam temperature in the jacket, $T_{\mathrm{j_{st}}}$, is determined as the boiling temperature corresponding to the partial pressure $P_{\mathrm{j_{st}}}$ in the jacket.

3.4. Model based supervisory

At every sampling period, the thermal flux limit capacities are determined for each utility fluid from the previous set of equations and according to the following considerations:

3.4.1. Glycol/water

Its maximum value corresponds to a zero flowrate (=0).

The minimum value $Q_{\mathrm{min_{gw}}}$ corresponds to the maximum flowrate, $F_{\mathrm{max_{gw}}}$, of the glycol/water stream available at the temperature T_{gw} (−15°C in practice). It is computed according to Eqs. (6) and (5).

3.4.2. Intermediate fluid

$Q\mathrm{max}_{\mathrm{if}}$ is determined from Eqs. (6), (8) and (11) for $F_{\mathrm{max_{if}}}$ corresponding to $F_{\mathrm{max_{st}}}$. In practice, $F_{\mathrm{max_{st}}}$ has been chosen in order to get a maximum temperature of 70°C. The minimum thermal flux $Q_{\mathrm{min_{if}}}$ corresponds to the case where only cold water is used as intermediate fluid, by taking T_{cw} as $T_{\mathrm{j_{in}}}$ and F_{cw} as F in Eqs. (6) and (8).

3.4.3. Steam

The maximum value $Q_{\mathrm{max_{st}}}$ is obtained for β=1 in Eqs. (7) and (14). To determine the steam temperature corresponding to the maximum flowrate, a non-linear function (Eqs. (7), (14) and (15)) has to be solved by an iterative procedure. The minimal thermal flux $Q_{\mathrm{min_{st}}}$ is obtained when the valve is closed ($Q_{\mathrm{min_{st}}} = 0$).

3.4.4. Strategy of supervision

The required thermal flux computed by the master controller (Q_{cont}) is compared to the limit capacities of the present fluid. If it exceeds these limits the appropriate changeover is performed. Moreover, when a changeover from water/glycol to the intermediate fluid or reciprocally is performed, an air-purge of the jacket is carried out before feeding the jacket with the new fluid. Let us notice that changeovers from steam to glycol/water or reciprocally are not authorized due to problem of thermal shocks.

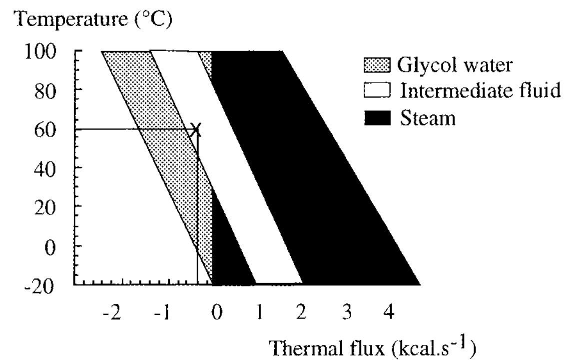


Fig. 2. Evolution of the thermal flux capacities for the different fluids.

Fig. 2 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. For example, the cross indicated on Fig. 2 corresponds to the case for which the reactor temperature is equal to 60°C and the required flux computed by the master controller Q_{cont} is equal to $-0.2\ \mathrm{kcal\ s^{-1}}$. As shown by Fig. 2, two fluids can be chosen: glycol water or the intermediate fluid. As said before, the priority is given to the fluid present in the jacket. On the other hand, if the fluid already present in the jacket is steam, a changeover to the intermediate fluid would be performed.

It is important to notice that, in comparison with most of the previous works, changeovers of fluids are not performed according to a predefined temperature alarm system but according to the physical capacity of the heat exchanges.

3.5. Computation of the thermal fluid flowrate

Once the right configuration has been chosen, the required thermal flux is then used in the model, in a slave-like loop, to evaluate the opening value of the control valve. The flux to be exchanged by the chosen thermal fluid (Eq. (6) for liquid fluid, Eq. (7) for steam) is computed by the master controller (Q_{cont}). Thus, contrary to the previous procedure (Section 3.4), the objective is to determine the flowrate of the fluid by using the equations given above.

In the case of the intermediate fluid, two operations have to be considered: without and with recycling of the intermediate fluid. In the first case (without recycling), this flowrate corresponds to the amount of injected steam in the cold water. The actual manipulated variable is the valve B opening degree computed according to the calibration characteristics of the valve which have been determined experimentally.

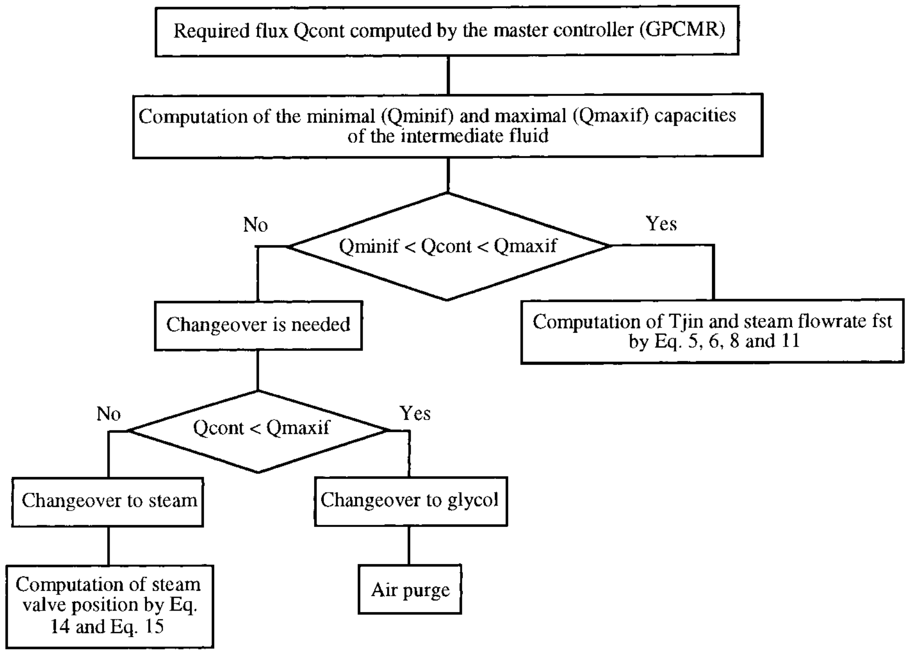


Fig. 3. Flow chart of the supervisory and control in case of the intermediate fluid (without recycling).

In the second case, a comparison between the calculated inlet temperature, T_{jin}, and the measured outlet jacket temperature T_{jout} allows to choose the fluid to be injected in the intermediate fluid and to determine the corresponding valve opening degree (valve A for water, valve B for steam). Moreover, in practice the flowrate of the intermediate fluid (F_{if}) is kept constant by a trap.

If $T_{\mathrm{jout}} \geq T_{\mathrm{if}}$ injection of cold water (valve A) is needed. The flow of fresh cold water (F_{cw}) to be introduced is given by

$$F_{\mathrm{cw}} = F_{\mathrm{if}} \frac{T_{\mathrm{jin}} - T_{\mathrm{jout}}}{T_{\mathrm{cw}} - T_{\mathrm{jin}}}. \tag{16}$$

If $T_{\mathrm{jout}} < T_{\mathrm{if}}$, the quantity of steam (valve B) to be introduced is given by

$$F_{\mathrm{st}} = F_{\mathrm{if}}.C_{p_{\mathrm{cw}}}.\frac{T_{\mathrm{jin}} - T_{\mathrm{jout}}}{[\mathrm{Lv} - C_{p_{\mathrm{cw}}}(T_{\mathrm{jin}} - T_{\mathrm{st}})]}. \tag{17}$$

A flow chart of the overall procedure is given in Fig. 3 for the case of the intermediate fluid present in the jacket without recycling.

4. Experimental results

To demonstrate the good performances of this new control methodology, different experiments have been carried out on the pilot plant reactor previously described. The reactor has been fed with 10 l of water at 21°C. This type of experiments, without heat released, is representative of a lot of fine chemistry operations like emulsifications, athermic reactions or crystallizations for example.

To get more readable figures, the maximum limit capacity for steam ($Q_{\mathrm{max_{st}}}$), which is in the range 4–5 kcal s^{-1}, is not plotted on the figures giving the evolution of the different fluxes.

The first experiment consists of controlling the temperature along the following profile:

- 1st phase: heating from 21°C to 45°C in 1500 s.
- 2nd phase: constant temperature set-point of 45°C during 2500 s.
- 3rd phase: cooling from 45°C to 30°C in 2500 s.
- 4th phase: maintain at 30°C for 500 s.

Fig. 4 shows time evolutions of the reactor temperature, the temperature set-point and the valve opening degree (the manipulated variable). The plotted valve opening degree (β)

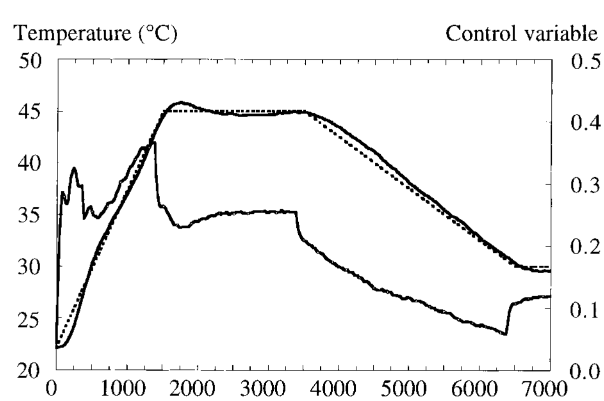


Fig. 4. Temperature and manipulated variable (first experiment without recycle).

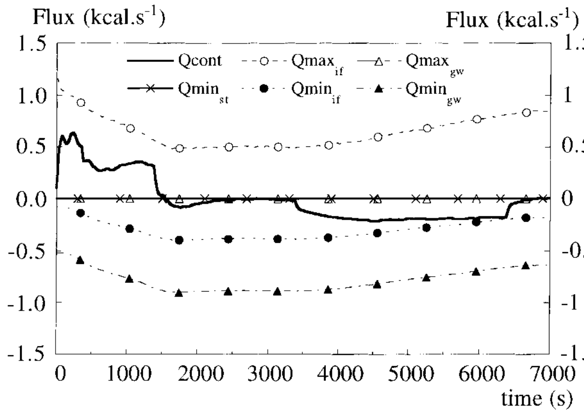


Fig. 5. Limits and control value of the thermal flux (first experiment without recycle).

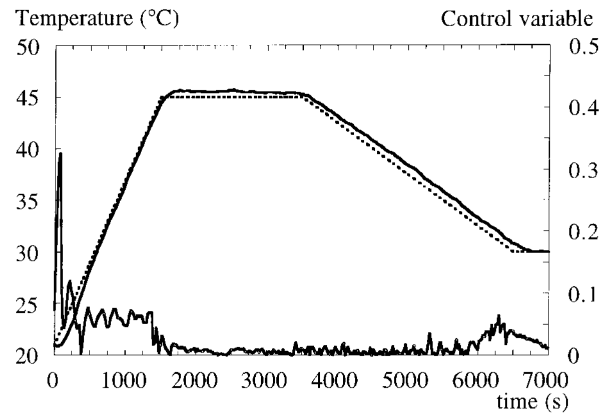


Fig. 7. Temperature and manipulated variable (second experiment with recycle).

corresponds to an experimental run performed without recycling of the intermediate fluid. In Fig. 5, time evolutions of the limit capacities for each fluid ($Q_{\max}$ and $Q_{\min}$) and of the thermal flux required ($Q_{\rm cont}$ computed by the controller) are plotted. This figure shows that the intermediate fluid is used during the entire profile. As soon as the constant temperature step is reached, the computed thermal flux becomes negative (Fig. 5). This example shows the double role of the intermediate fluid which can be used for both heating and cooling. In this experiment the valve opening degree (β) always corresponds to the valve B which control steam injection in cold water. Fig. 6 gives the evolutions of the inlet and outlet jacket temperature. As the intermediate fluid is the only fluid used, the inlet temperature corresponds to the intermediate fluid temperature obtained after the mixer.

The second experiment run deals with the same desired temperature profile but with recycling of the intermediate fluid. Fig. 7 gives the time evolution of the reactor temperature, the temperature set-point and the actual manipulated variable (β). In Fig. 8, time evolutions of the limit capacities for each fluid and of the thermal flux required

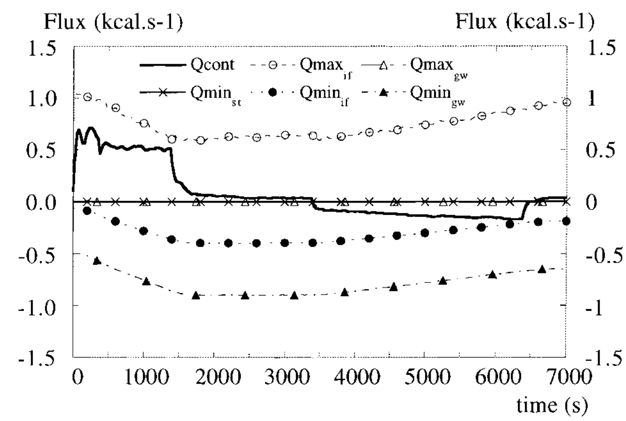


Fig. 8. Limits and control value of the thermal flux (second experiment with recycle).

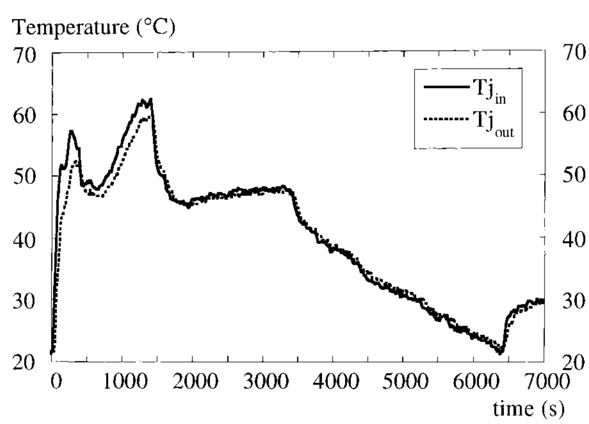


Fig. 6. Inlet and outlet jacket temperatures (first experiment without recycle).

($Q_{\rm cont}$) computed by the controller are plotted. These two plots show that the intermediate fluid is used during all the profile. As for Fig. 5, as soon as the constant temperature step is reached, the computed thermal flux becomes negative (Fig. 7). As described in Section 3.5, for this experiment, the valve opening degree (β) concerns both valves A and B depending on the fact that the inlet jacket temperature has to be increased or decreased.

According to Figs. 5 and 8, we can notice that the evolution of the computed thermal flux is similar in the two cases with and without recycling of the intermediate fluid. On Figs. 9 and 10 a comparison of steam and cold water consumptions for the two experiments has been plotted. The figures clearly show that recycling allows high energy savings. In addition, this arrangement enables a good adjustment of the hot water temperature at the jacket inlet by feeding small amounts of steam or cold water as a function of the required thermal flux. Figs. 4 and 7 show that in both cases (with and without recycling) the reactor temperature follows perfectly the set-point temperature profile. Moreover, a very soft evolution of the manipulated variable is obtained.

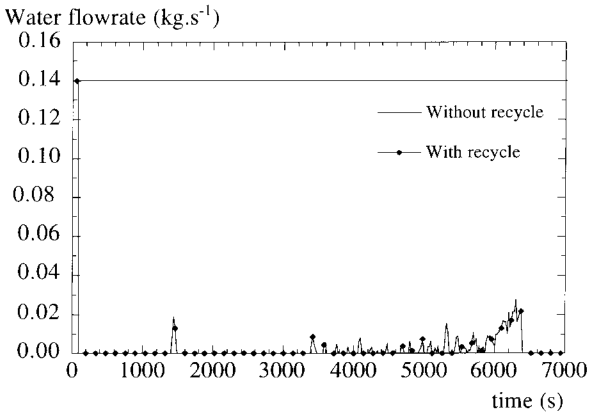


Fig. 9. Comparison of cold water consumption with and without recycling of the intermediate fluid.

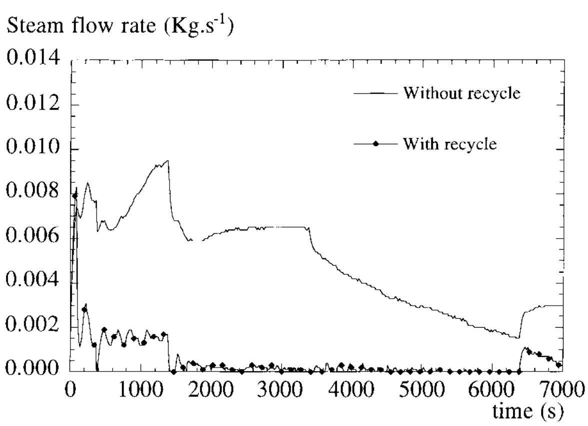


Fig. 10. Comparison of steam consumption with and without recycling of the intermediate fluid.

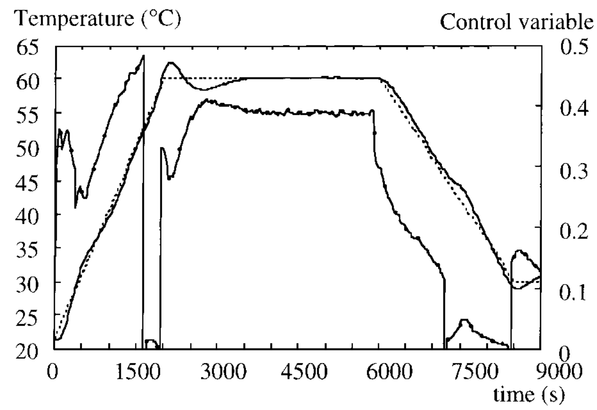


Fig. 11. Temperature and manipulated variable (third experiment).

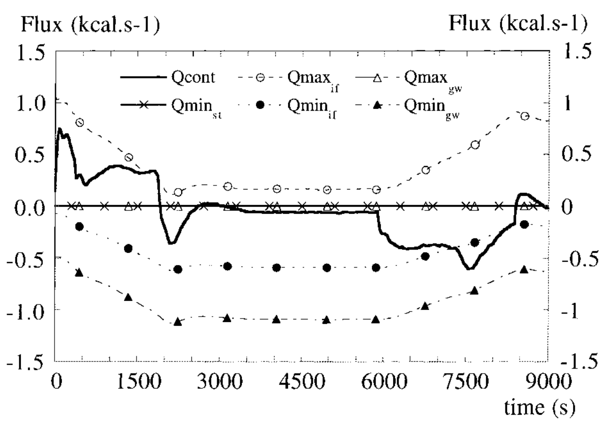


Fig. 12. Limits and control value of the thermal flux (third experiment).

All these points demonstrate the efficiency and the good performances of the developed control strategy. To show the accuracy of this strategy particularly for supervisory performance, another experiment has been carried out at a different temperature set-point of 60°C with the following desired profile:

- 1st phase: heating from 21°C to 60°C in 2000 s.
- 2nd phase: constant temperature set-point of 60°C during 4000 s.
- 3rd phase: cooling from 60°C to 30°C in 2500 s.
- 4th phase: we maintain constant temperature set-point of 30°C for 500 s.

Fig. 11 shows the evolutions of the temperature in the reactor, the temperature set-point and the valve opening degree (without recycling). A good tracking performance of the cascaded model based controller can be noticed.

Fig. 12 shows the evolutions of thermal flux limits for each utility fluid and the thermal flux (Q_{cont}) computed by the first loop controller (GPCMR). Compared to the previous experiments (Figs. 5 and 8), all the different utility fluids have to be used. In particular, at the end of the heating phase (1500 s), steam is required. The heating capacity of the intermediate fluid is no longer sufficient to achieve the desired heating demand. Similarly, during the cooling phase (around 8000 s), the higher cooling rate implies a changeover from the intermediate fluid to glycol/water. This demonstrates the efficiency of the developed methodology in cases of changeovers of fluids.

Finally, to show the behaviour of this strategy in face of thermal disturbances, another experiment has been carried out with the following desired profile:

- 1st phase: heating from 18.5°C to 40°C in 1500 s.
- 2nd phase: constant temperature set-point of 40°C during 2500 s.
- 3rd phase: cooling from 40°C to 30°C in 2500 s.
- 4th phase: we maintain constant temperature set-point of 30°C for 500 s.

Two litres of hot water at 80°C is introduced during the maintenance phase (between 1500 and 3000 s) with a feeding rate of 5 kg h^{-1}. This allows to provoke a sudden and difficult-to-predict heat effect in order to simulate an exothermic reaction.

Fig. 13 shows the evolutions of the temperature in the reactor, the temperature set-point and the valve opening

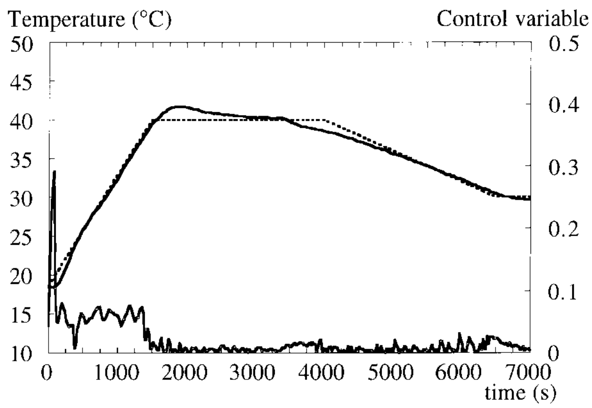


Fig. 13. Temperature and manipulated variable (experiment with artificial disturbance).

degree (with recycling). The heating and cooling phases are satisfactorily achieved and a good tracking performance of the cascaded model based controller can be noticed.

During hot water feeding, firstly an overshoot (leading to a maximum gap of 1.7°C) is observed. Then, the controller reacts and computes a cooling action which brings the reactor temperature back to the set-point. At the end of feeding, as the thermal effect is stopped suddenly, the temperature becomes inferior to the set-point value due to the cooling action. The reaction of the controller is not rapid enough to avoid initial overshooting and final overcooling. Nevertheless, a rapid calculation shows that without any action of the controller the temperature would have reached a value of 46.7°C.

Fig. 14 shows the evolutions of thermal flux limits for each utility fluid and the thermal flux (Q_{cont}) computed by the first loop controller (GPCMR). It is interesting to examine the behaviour of this controller during the disturbance. As soon as the heating effect appears, the computed thermal flux begins negative. At the end of hot water feeding, the thermal flux becomes positive again. Nevertheless, the reaction of the controller is not rapid enough to avoid initial overshooting and final overcooling.

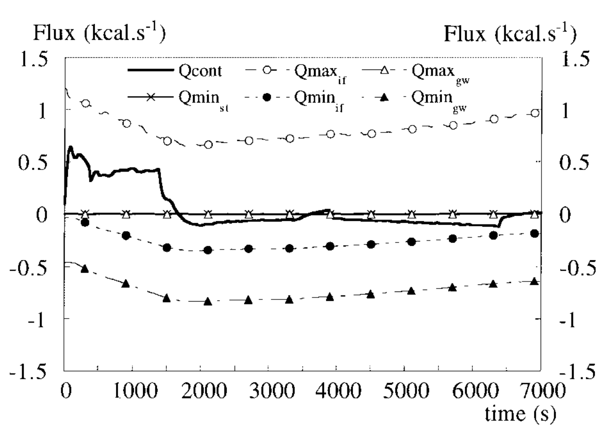


Fig. 14. Limits and control value of the thermal flux (experiment with artificial disturbance).

In this work, the input–output model used in the GPCMR controller is based on Section 3.1 and nothing is done to take into account sudden heat effects. Compensation of these effects is only made by adaptation of the model parameters. Studies are now in progress to develop such heat estimators in order to improve the controller behaviour when it has to face heat effects.

5. Conclusion

A new methodology for 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 computed by the master controller is then used in a model-based supervisory structure which, according to the limit capacities of the different fluid configurations, allows to choose the "right" one. The model equations are then used to compute the manipulated variable (valve position).

In this paper, this methodology has been applied to a new heating–cooling system which takes advantage of the large heating (cooling) capabilities of steam (glycol/water) when rapid heating (cooling) is needed. On the other hand, for normal operating conditions, the use of an intermediate fluid circulating at a sufficiently rapid flowrate to ensure good heat transfer coefficients is preferred.

The application of such a methodology to a pilot plant build around a 16 l glass-lined jacketed reactor has been presented. One of the main interests of this methodology is the implicit management of several fluids by the control system which associates a control algorithm with a model-based supervisory procedure.

This strategy is not limited to the heating–cooling system presented in this paper, but may be extended to any system whatever the number of fluids is.

6. Nomenclature

A	heat exchange area	m^2
C_p	heat capacity	$kcal\ kg^{-1}\ K^{-1}$
cvs	steam valve characteristic	$kg^{1/2}\ m^{1/2}$
F	flowrate	$kg\ s^{-1}$
Lv	latent heat	$kcal\ kg^{-1}$
P	pressure	$kg\ m^{-1}\ s^{-2}$
Q	thermal flux	$kcal\ s^{-1}$
T	temperature	K
T_j	jacket temperature	K
U	heat transfer coefficient	$kcal\ s^{-1}\ m^{-2}\ K^{-1}$

Greeks letters

β	valve opening degree

Subscripts

air	air
cw	cold water
cont	controller
if	intermediate fluid
in	inlet
gw	glycol water
out	outlet
st	steam

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