A CONTROL SYSTEM FOR A PILOT BATCH POLYMERIZATION REACTOR

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ABSTRACT : *In this article several control schemes for a pilot scale polymerization reactor are proposed and one of them is selected as the most suitable design. The performances of proposed schemes have been compared through computer simulations. The controllers are PID and chosen reaction is polymerization of methyl methacrylate which is highly exothermic.*

KEY WORDS : *Polymerization, Batch reactor, Modeling, Gel effect, PID controller.*

INTRODUCTION

In chemical reactors, temperature is the most important parameter that should be controlled. Due to the changes in operating conditions, controlling of a batch reactor is more difficult than a continuous one. In a batch reactor the reactants should be heated initially and after the reaction starts, heat has to be removed from the system for exothermic reactions. After decrease in the reaction and heat generation rates it may become necessary to introduce heat to the system. Therefore, the control system should be capable of heating and cooling the reactor. Usually for investigating the effects of different parameters on the reaction rate and obtaining the necessary data for designing an industrial reactor, a pilot unit is required. In this paper four different control schemes for a pilot reactor have been proposed. These schemes are compared through simulations and one scheme is recomended as the best design. The polymeri-

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zation of methyl methacrylate (MMA) which is highly exothermic is considered in the simulation studies.

PROCESS MODEL

In free radical polymerization of MMA the reaction proceeds by radical formation in presence of an initiator. At a specified conversion level, due to the gel effect the rate of heat generation increases drastically and after that it decreases very rapidly.

In Fig. 1 the rate of heat generation due to the reaction is shown as a function of time.

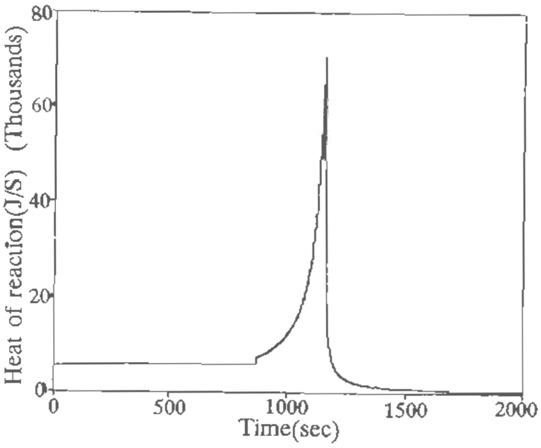

Fig.1: The rate of heat generation of MMA polymerization.

The kinetic model proposed by *Ross* and *Laurence* [1], are used for simulation studies and detailed information are provided in reference [2].

The reactor is equipped with a jacket for heat transfer and is shown schematically in Fig. 2.

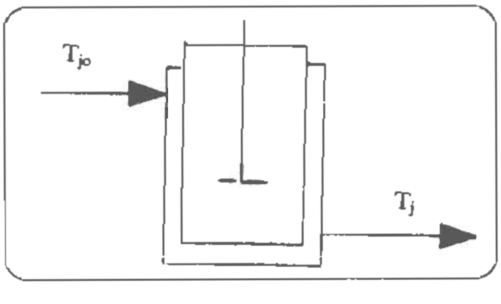

Fig. 2: Schematic diagram of the reactor.

If the exit temperature for the heat transfer fluid is shown by T_j , and that of the reactor by T, and rate of heat generation by Q, then process transfer function is given by [2].

$$T(s) = \frac{1}{\tau_p s + 1} [T_j(s) + a\, Q(s)] \qquad (1)$$

The transfer function of the reactor jacket, obtained from the energy balance around the jacket, is given below [2]:

$$T_j(s) = \frac{1}{\tau_j s + 1} [bT(s) + c\, T_{jo}(s)] \qquad (2)$$

T_{jo} indicates the temperature of the fluid entering the jacket and definitions of other terms a, b, c are given in reference [2]. The block diagram of the process is shown in Fig. 3.

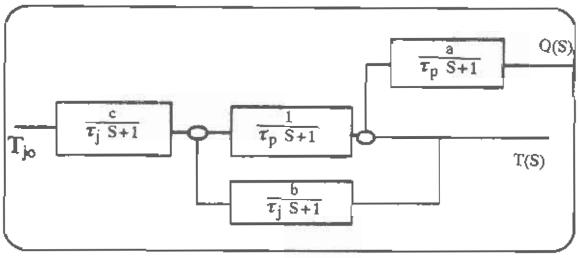

Fig. 3: Process block diagram.

The reactor size and other data are given in Table 1. The heat transfer fluid is Dowtherm. Since a pilot scale reactor is considered, the heat transfer fluid circulates through a closed loop which indeed prevents wasting the heat transfer fluid.

CONTROL SCHEMES

In this part four control schemes for controlling reactor temperature are proposed. The performances of the schemes are compared through computer simulations. Differential equations describing the system dynamics, obtained from mass and energy balances, are solved with controller equation simultaneously. The *Runge-Kutta* method is used for solving the equations and the computer program is written in *Quick Basic.*

Table 1: The data of the simulated system.

Rotation rate of reactor mixer	3 cycles/sec
Rate of heat transfer fluid (Dowtherm A) in the jacket	2kg/sec
Monomer to water ratio in the reactor	0.25
Initial concentration of initiator, (AIBN)	0.02mol/L
Suspension volume in the reactor	100L
Overal heat transfer coefficient between jacket and reactor	$647 J/S.m^2.°C$
Heat transfer area between reactor and jacket	$1m^2$
Type of jacket's baffle	Spiral baffle
Rate of cooling water in the heat exchanger	1kg/sec
Heat transfer area of the exchanger	$2.5m^2$
Volume of the cool fluid source	100L
Volume of the hot fluid source	50L
Power of the heating element	30kW

CONTROL SCHEME I

This scheme is shown in Fig. 4. As can be seen from Fig. 4, a cascade control strategy is used. The slave controller is a P type and the master controller is a PID type. If instead of a cascade control system a simple feedback control loop is used, the control would be unsatisfactory and oscillations remain in the reactor temperature. In this design a three-way control valve is used which actuates in the range of 4-12mA.

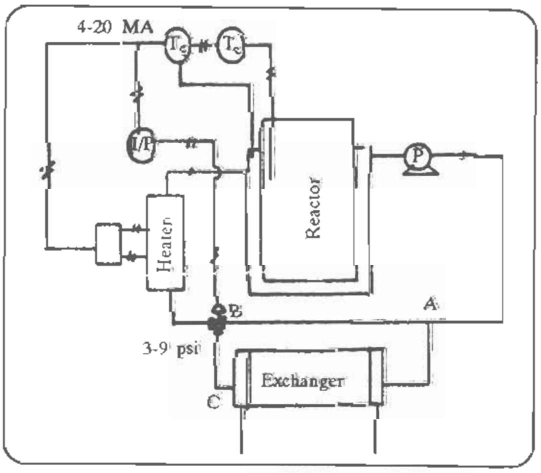

Fig. 4: Schematic diagram of control scheme I.

When controller output is 4mA, the line AC is fully open. As controller output increases, the flow rate in the line AC decreases and consequently the flow rate in the line AB increases. At 12mA, the line AC is fully closed and the line AB is fully open. For heating the system, an electrical element is used which has its maximum power when the controller output signal is 20mA and zero power at 12mA. The initial temperature of the reactants is 25°C and it is intended to control the reactor temperature at 90°C. The simulation result is shown in Fig. 5. For tuning the controller the integral of time weighted absolute value of the error is used.

$$PI = \int_{0}^{\infty} t\,|e|\,dt \qquad (3)$$

The optimum controller parameters and the minimum value of the performance index for each design are given in Table 2. To prevent the controller windup, the integration is stopped as soon as the actuator becomes saturated [3].

As can be seen from Fig. 5, there is one overshoot at the begining of the gel and one undershoot after the gel. The overshoot is due to the limited cooling effect of the heat exchanger and lack of the source of cold heat transfer fluid. The undershoot is due to lack of source of hot heat transfer fluid and the fact that the electrical heater is off during the cooling period and it takes time to heat it.

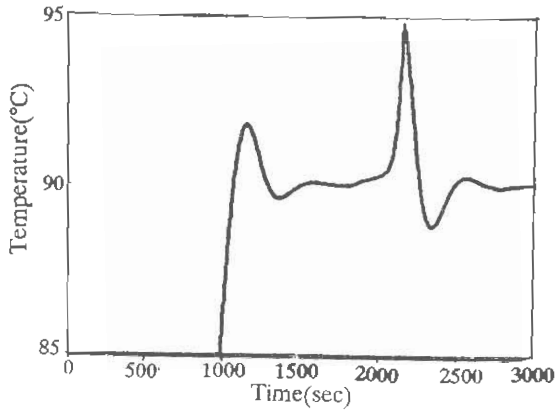

Fig. 5: Reactor temperature vs. time for control scheme I.

CONTROL SCHEME II

The schematic diagram of this design is shown in Fig. 6.

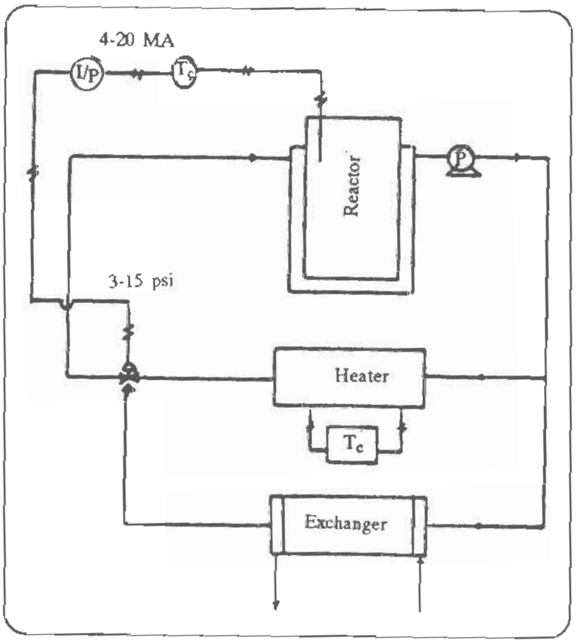

Fig. 6: Schematic diagram of control scheme II.

The difference between this scheme and the previous one is the addition of a hot heat transfer fluid source whose temperature is controlled by a thermostat. The advantage of this scheme compared to the former one is the availability of a hot fluid source which can supply heat faster. Also it should be mentioned that in this design a simple feedback PID loop is used which is preferable to scheme I from economical point of view. Simulation result is shown in Fig. 7.

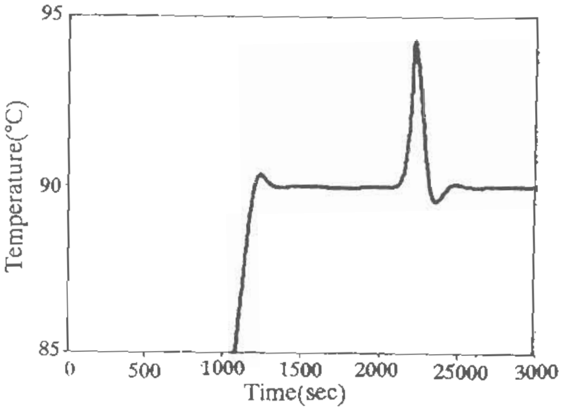

Fig. 7: Reactor temperature vs.time for control scheme II.

As can be seen the undershoot after the gel is decreased which is the consequence of utilizing the hot fluid source. Incidently the first overshoot is also decreased, because the heating system is out of the control loop during the cooling period.

CONTROL SCHEME III

As can be seen from the simulation result of control scheme II, due to hot fluid source the undershoot after the gel, is decreased but the overshoot before the gel is still significant. To solve this problem a cool fluid source is added to the scheme II which enters the control loop by the action of a solenoid valve, if the control output signal exceeds a given limit. At this situation the heat exchanger and cool fluid source are connected in series. The schematic diagram of this scheme is shown in Fig. 8.

In simulation studies, the system is designed in such a way that if the difference between the desired temperature and reactor temperature exceeds 0.5°C, the solenoid valve is actuated and the cool fluid source enters the control loop. Simulation result is shown in Fig. 9.

As it is evident, the overshoot before the gel is decreased significantly which is due to the effect of the cool fluid source.

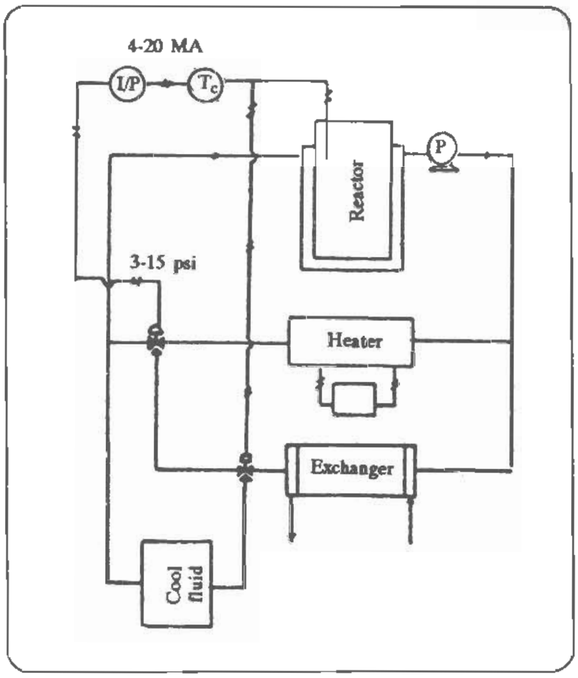

Fig. 8: Schematic diagram of the control scheme III.

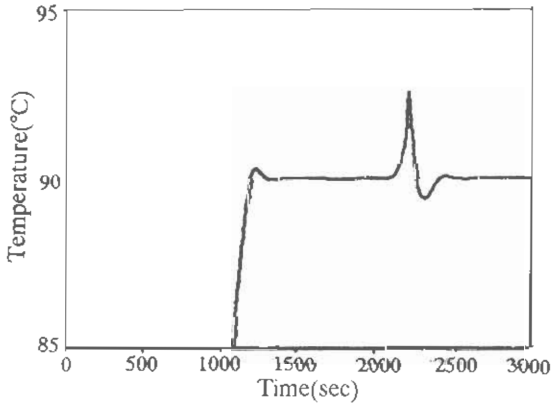

Fig. 9 : Reactor temperature vs.time for the control scheme III.

CONTROL SCHEME IV

In the previous design there exists a solenoid valve which is actuated when the error signal exceeds a specified threshold.

It is preferable to design a system that works automatically and it is not needed to specify the error threshold. The control scheme IV is such a design and is shown in Fig. 10. This control design has three control valves and one solenoid. The ranges in which control valves actuate are shown in Fig. 10. The solenoid valve is actuated when the control output after the I/P converter is 7psi. The control configuration is a cascade type and the optimum value of the controllers' parameters are given in Table 2. Simulation result is shown in Fig. 11.

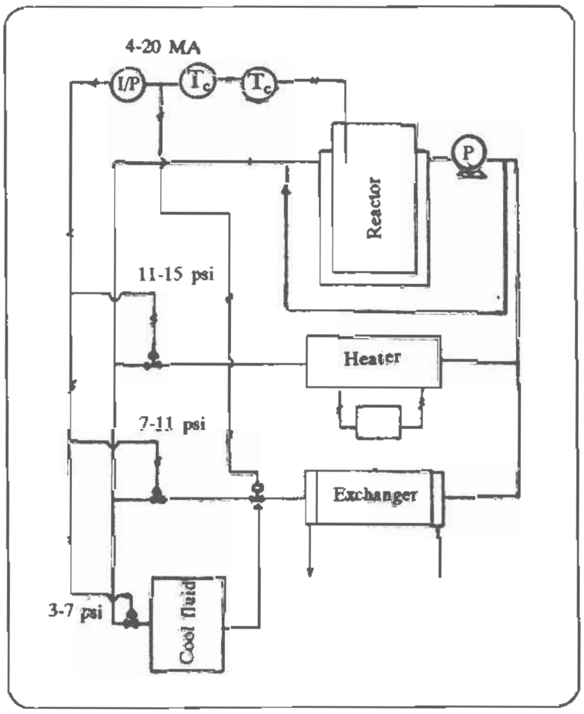

Fig. 10: The schematic diagram of the control scheme IV.

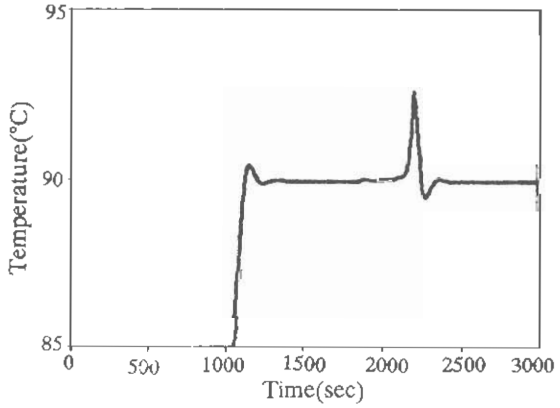

Fig. 11: Reactor temperature vs.time for the control scheme IV.

As can be seen from the simulation results the performance of this scheme is better than the others. The value of the preformance index for this scheme which is the lowest one is given in Table 2. It should be mentioned that, although this scheme has two additional control

Table 2: Controllers parameters and the minimum values of the objective function for different schemes.

	K_{cm}	τ_i	τ_d	K_{cs}	$\int t\|e\|dt$	Overshoot[1] (°C)	Overshoot[2] percentage
Scheme I	15	55	34	48	154.478×10^5	4.9	–
Scheme II	270	50	20	–	152.097×10^5	4.1	16
SchemeIII	270	50	17	--	148.820×10^5	2.5	50
Scheme IV	45	25	9	38	147.348×10^5	2.4	51

1 = Overshood due to gel effect.
2 = Percentage of overshoot reduction compared to scheme I.
e = Error signal (setpoint temperature-reactor temperature).
K_{cm} *= Gain of master controller.*
τ_i *= Integral time.*
τ_d *= Derivative time.*
K_{cs} *= Gain of slave controller.*
τ_p *= Reactor time constant.*
τ_j *= Jacket time constant.*

valves and one controller compared to the control design III, there is not a significant difference between the performances of these schemes.

CONCLUSIONS

Simulation results show that schemes III and IV have good performances. The performance of the scheme IV is slightly better than the scheme III at the expense of two additional control valves and one controller. Since the difference is not appreciable, the additional investment is not justified and the control scheme III is recommended as the most suitable design.

REFERENCES

[1] Ross, R.T., and Laurence, R.L., "*Gel effect and free volume in the bulk polymerization of methyl methacrylate*". AIChE Symp. Series, 72, 160 (1976).

[2] Shahrokhi, M., and Parvazinia, M., "*The temperature control of batch polymerization reactors*". Iranian Journal of Polymer Science & Technology, 4(2), (Aug. 1991).

[3] Seborg, D.E., *Process dynamics and control. John Wiely & Sons,* (1989).