A Control Configuration for Temperature Control of a Cooling Crystallizer Based on a Two-level-model Predictive Control

S. Mortazavi-Manesh* **and W. Y. Svrcek**
Department of Chemical and Petroleum Engineering, University of Calgary
2500 University Drive NW Calgary AB T2N 1N4, Canada

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A two-level-model-predictive-control configuration is proposed that incorporates the dynamics of a crystallizer unit in order to track the required temperature cooling trajectory. Dynamic matrix control has been successfully used to control the crystallizer temperature by manipulating both heater and cooler units. The performance of the model predictive control has been evaluated by comparing its performance to a conventional PI control configuration. The results demonstrated excellent and consistent cooling temperature tracking performance by the dynamic matrix controller.

Key words:
Crystallization, cooling crystallization, model predictive control

Introduction

Crystallization is one of the separation processes in the chemical industry.[1] In a typical crystallizer operation, temperature control is the key to the product properties. Fig. 1 illustrates the general thermodynamic phase behavior of a solute-solvent. Fig. 1 shows that any liquid from a stable zone with a temperature and a composition below the solubility curve is unsaturated and stable. Cooling a liquid from the stable zone to a temperature and composition on the solubility curve results in a saturated solution in equilibrium with the solid phase, if present. Further cooling results in a solution state that the composition of the liquid is greater than the equilibrium composition at the given temperature. Any liquid with a composition and temperature above the solubility curve is not in thermodynamic equilibrium and thus is supersaturated. In this region, nucleation sites are necessary to initiate the formation of a solid phase from a supersaturated liquid. Theoretically, if one could suppress all nucleation sites, the liquid could exist as a stable supersaturated liquid even though it would not be in thermodynamic equilibrium.[2] The region between the solubility curve and stability limit curve is called the metastable zone. In the region above the metastable zone, the presence of nucleation sites is not a requirement for the formation of a solid phase, as spontaneous nucleation and formation of solid phase takes place; therefore this region is called an unstable zone. Basically, in order to produce a solid phase a crystallizer must operate above the solubility curve. However, since production of a large number of small particles is not desirable, the operating region is restricted to the metastable zone. Note, one should avoid operating the crystallizer in the unstable zone. Staying within the metastable zone typically leads to crystallizations dominated by crystal growth and reduced secondary nucleation within the ongoing crystallization.[3,4] That is, crystallization within the metastable zone results in a defined crystal growth rate, a desired particle size, obtaining narrow particle size distributions, and reducing the risk of producing a non-useable polymorph.[5–7]

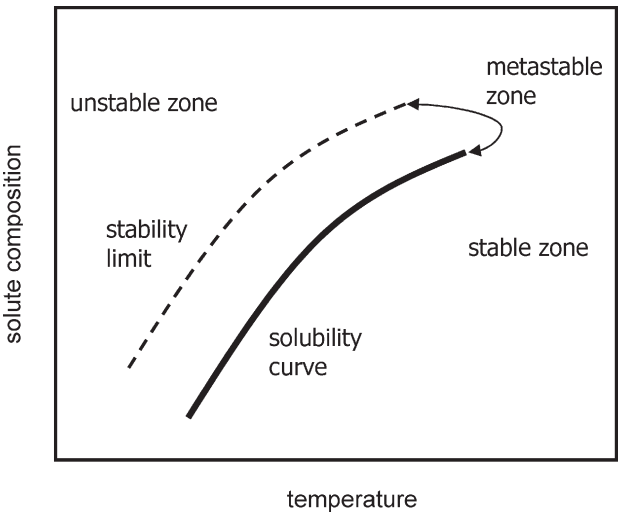


Fig. 1 – *Phase behavior of a solute-solvent system*

One approach to control a bath crystallizer is to follow a temperature profile in the metastable zone.[8] An alternative approach is to follow a supersaturation profile in the metastable zone.[9,10]

In order to utilize either of the above control policies a DMC has been developed and imple-

*Corresponding author: smortaza@ucalgary.ca

mented. Dynamic matrix control (DMC) is a variant of model predictive controller (MPC) which was developed by Culter and Ramaker[11] of Shell Oil Co. and has been widely accepted industrially mainly in the oil and petrochemical industry.[12,13] The success of DMC in industry is the result of DMC's ability to deal with multivariable processes.

MPC strategies have already been used for controlling the temperature control of batch crystallizers.[14,15] The goal of this study is to investigate the performance of a two-level-DMC controller. In this study, in order to save more energy, the jacket water is recycled which is different from the previous setups in which the hot and cold streams are mixed to regulate the temperature of the jacket water of the crystallizer.[14,15]

The basic theory of DMC control is presented in section two of this article. The crystallizer unit is described in section three and then the experimental results are presented in section four followed by the discussions and conclusions in sections five and six.

DMC theory

The control calculations of a MPC strategy are based on current and previous process responses and previous values of the implemented inputs, current measurements and future predictions of the process variables. The future predictions are based on empirical dynamic models. In the case of the DMC strategy, those empirically obtained models are typically multivariable step response models. The objective of the DMC strategy is to determine the future changes in manipulated variables in such a way that the predicted process variables move to the desired targets in an optimal manner; in other words, at the current sampling time the DMC controller uses an optimization algorithm to calculate M future manipulated variable moves (control horizon) in such a way that the predicted process variable reaches the target after P sample times (prediction horizon). However, only the first move is implemented at each sample time so that the measurements could be updated and the optimization algorithm could be repeated at each sample time.

In a process with two manipulated variables and one process variable the step response model for the DMC is defined by eq. (1):[11,16–18]

$$y(\theta+1) = y_0 + \\ + \sum_{i=1}^{2} \sum_{j=1}^{N_i-1} S_{i,j} \Delta u_i(\theta - j + 1) + S_{i,N_i} u_i(\theta - N_i + 1) \quad (1)$$

Where, $y(\theta+1)$ is the process variable at $(\theta+1)$ sample time. y_0 is the initial value of the process variable and $\Delta u_1(\theta - j + 1)$ and $\Delta u_2(\theta - j + 1)$ represent the changes in manipulated variables from one sample time to the next. $S_{1,j}$ and $S_{2,j}$ are the coefficients of the step response model. The choice of the number of the coefficients and the sample time depend on the process dynamics.

A quadratic objective function J can be defined by eq. (2)

$$\min_{\Delta U} J = \hat{E}^T Q \hat{E} + \Delta U^T R \, \Delta U \quad (2)$$

Where, $\hat{E}$ is a $P \times 1$ vector which represents the error between the predicted values and the reference trajectory P sample time into the future ΔU a $2M \times 1$ vector representing the M movements of manipulated variables. **Q** and **R** are the weighting matrices used to weight the most important elements of E or ΔU.

The Model Predictive Control law that minimizes the objective function in eq. (2) can be calculated analytically using eq. (3).

$$\Delta U(k) = K_C \hat{E} \quad (3)$$

In which K_C is a $2M \times P$ matrix given by eq. (4)

$$K_C = (S^T Q S + R)^{-1} S^T Q \quad (4)$$

And the dynamic matrix **S** is defined by eq. (5)

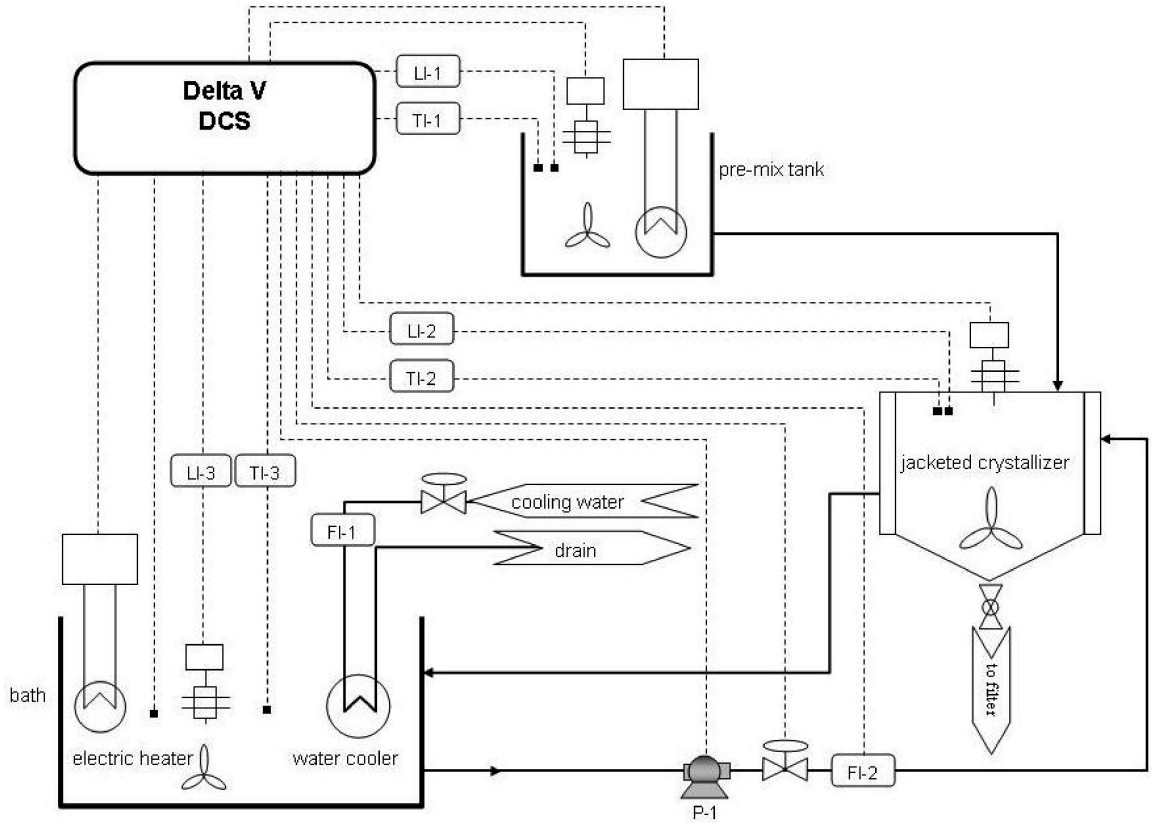
$$\mathbf{S} = \begin{bmatrix} S_1 & 0 & \dots & 0 \\ S_2 & S_1 & 0 & \\ \vdots & \vdots & \ddots & 0 \\ S_M & S_{M-1} & \dots & S_1 \\ S_{M+1} & S_M & \dots & S_2 \\ \vdots & \vdots & \ddots & \vdots \\ S_P & S_{P-1} & \dots & S_{P-M+1} \end{bmatrix} \quad (5)$$

Where $\mathbf{S}_i$ is a 1×2 vector of step-response coefficients for the i-th time step as shown in eq. (6).

$$\mathbf{S_i} = [S_{1,i} \; S_{2,i}] \quad (6)$$

Description of the crystallizer

Fig. 2 is a schematic of the batch crystallization mini pilot built for this study. The pre-mixer tank is used to prepare the solution by dissolving solute in the water and heating the solution to the desired temperature. The solution is then transferred to the jacketed crystallizer. The crystallizer temperature trajectory is controlled by circulating water through the crystallizer jacket. The temperature of the jacket water is regulated in the water



F i g . 2 – *Crystallizer unit*

bath using both an electrical heater and a water cooler that are immersed in the water bath. All three vessels are equipped with stirrers to provide a uniform temperature and higher heat transfer rates and to keep the crystals in the solution. The speed of the stirrers can be manually adjusted using the stirrer drive motors mounted on each vessel and these motors can be turned off and on via the DCS. Both the pre-mix tank and the water bath are equipped with digitally controlled water immersion heaters, and the temperatures of the vessel contents are measured using thermocouples. The flow rate of the circulating water inside the crystallizer jacket and the flow rate of the cooling water are both controlled using electrically operated valves. The flow rates of the cooling water and the circulating water are measured using rotary flow meters. In order to maintain the vessel's liquid level, indicators are provided.

The unit is equipped with DeltaV DCS 7.2 which has one active controller with five cards each having 8 channels.

For the purposes of this study, the DMC control software for the crystallization unit has been developed using Visual Basic 6.0. This software was directly linked to the Delta V and the developed software package considers the process variables as inputs and manipulated variable values as outputs.

For this study the crystallization of potassium chloride was performed. The solubility data for potassium chloride in water as the function of the temperature was available.[19] The literature did provide the width of metastable zone of the solutes in aqueous solutions.[1,19]

Results

Fig. 3 is a schematic of a two-level-DMC. The inside DMC is a slave single-input-multiple-output, SIMO, DMC that was implemented to control the water bath temperature. Here, the terms input and output are considered with respect to the controller not to the process. The SIMO DMC uses the bath temperature as the process variable and manipulates both the cooling water flow rate setpoint and the water bath electrical heater input. Note, there is a slave PI controller for the cooling water flow rate whose setpoint comes from the DMC. The dynamic behaviour of the bath can be represented by twostep-response models for the bath temperature response to step changes in heater duty and to the cooling water flow rate setpoint. The time constant and process delay of the water bath temperature response to the step changes in the cooling water flow rate setpoint and heater duty are shown in Table 1.

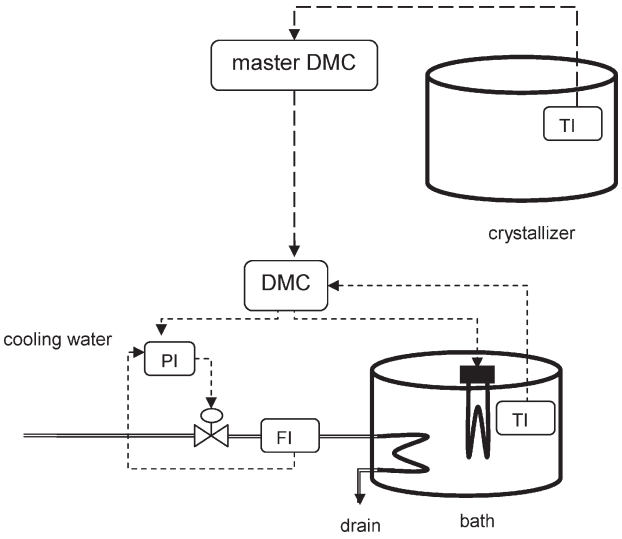


Fig. 3 – *Two-level DMC configuration for crystallizer temperature control*

Table 1 – *Process delay, time constant and gain of bath temperature response to the step changes in the cooling water flow rate and heater duty*

Step change	Delay, t_d/s	Time constant, t_c/s	Gain
heater duty	8	536	0.73
cooling water flow rate setpoint	8	508	−1.98

The following constraints are included in the SIMO DMC. The values greater than the maximum levels or less than the minimum levels of the constraints are considered equal to the maximum or the minimum levels of the constraints, respectively.

$$0 \leq \text{heater duty} \leq 100\ \% \tag{7}$$

$$0 \leq \text{cooling water flow rate setpoint} \leq \leq 5.00 \cdot 10^{-5}\ \text{m}^3\ \text{s}^{-1} \tag{8}$$

$$|\Delta(\text{setpoint of the cooling water flow at each sample time})| \leq 0.67 \cdot 10^{-5}\ \text{m}^3\ \text{s}^{-1} \tag{9}$$

The jacketed crystallizer vessel temperature is controlled by the water that flows through the jacket of the crystallizer. The jacket water temperature is regulated in the water bath vessel to a maximum allowable operating temperature of 60 °C. A two-level controller is implemented in which a master controller manipulates the water bath temperature setpoint in order to control the crystallizer vessel temperature. DMC and PI controllers are implemented to control the crystallizer vessel temperature and their performance is compared. A Master single-input-single-output, SISO, DMC has been implemented in which the crystallizer temperature is the process variable and manipulated variable is the setpoint of the slave DMC which is temperature setpoint of the water bath vessel. The dynamic behaviour of the crystallizer can be represented by a step response model which relates the crystallizer temperature response to step changes in the setpoint of the water bath temperature. Since the heater power can be changed easily and fast over the whole range of 0 to 100 %, a small penalty on the changes of the heater power is chosen for the slave DMC. However, the objective is to limit the changes of the setpoint of the cooling water flow rate in order to limit the load on the control valve therefore a larger penalty for the changes of the setpoint of the cooling water flow is considered for the slave DMC. In addition to obtain a fast response from the slave controller, the penalty of the error can be increased. In the case of the master DMC, the unit value is considered for both **Q** and **R**. The time constant and process delay (dead time) of crystallizer temperature response to the step changes in the bath temperature setpoint are shown in Table 2. The parameters for the DMC used to control the bath content temperature are provided in Table 3.

The constraint that is included in the master DMC is that the water bath temperature

$$\text{setpoint} \leq 55\ ^\circ\text{C} \tag{10}$$

Table 2 – *Time constant and process delay of crystallizer temperature response to the step changes in the water bath temperature setpoint from 30 °C to 40 °C*

Step change	Delay, t_d/s	Time constant, t_c/s	Gain
water bath temperature setpoint	91	1120	0.95

Table 3 – *DMC parameters*

	DMC for the bath temperature control loop	DMC for the crystallizer temperature control loop
sample time, θ/s	4	7
number of coefficients, N	150	170
control horizon, M	4	3
prediction horizon, P	9	25
Q	4	1
R	for heater = 0.01 for cooling water = 25	1

The performance of the two-level DMC has been tested via a series of step changes and ramps in the setpoint of the crystallizer temperature. The results of these setpoint tracking tests of the two-level DMC are shown in Fig. 4. The integral square error, ISE, of MPC used for controlling the crystallizer temperature is provided in Table 4. The control actions for the MPC for the crystallizer temperature loop are shown in Figs. 5, 6 and 7.

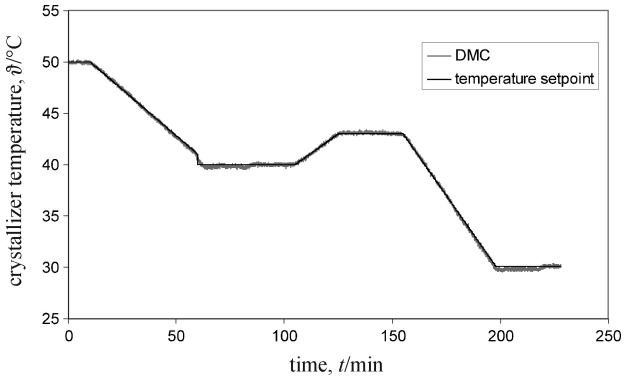


Fig. 4 – *Setpoint tracking test of DMC used in crystallizer temperature control loop*

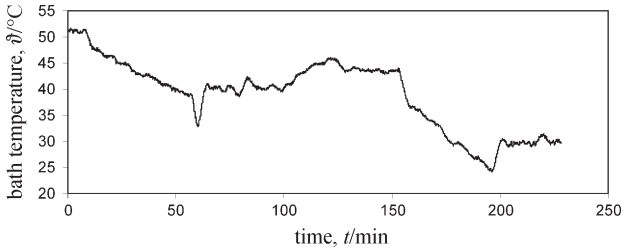


Fig. 5 – *Water bath temperature in setpoint tracking test of DMC used in crystallizer temperature control loop*

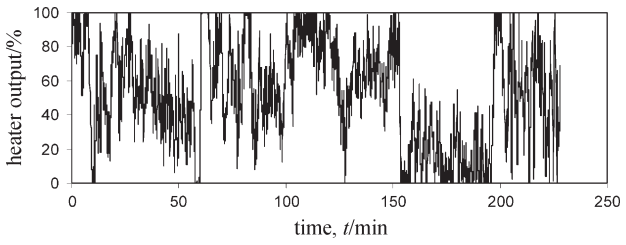


Fig. 6 – *Heater duty in setpoint tracking test of DMC used in crystallizer temperature control loop*

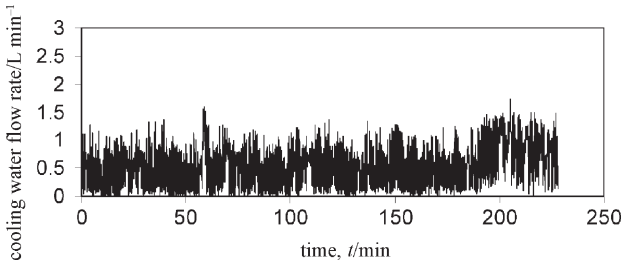


Fig. 7 – *Cooling water flow rate in setpoint tracking test of DMC used in crystallizer temperature control*

Table 4 – *Integral square error, ISE, of DMC and PI control strategy for crystallizer temperature control loop*

	ISE
DMC	325.19
PI	788.5

The results of the DMC have been compared with those of a cascade PI configuration; Fig. 8. Two PI controllers regulate the water bath temperature by manipulating water bath electrical heater duty and the setpoint of the PI flow controller. A master PI controller manipulates the setpoint of the water bath control loop to control the crystallizer vessel temperature trajectory. The PI parameters have been tuned using the auto tune variation technique,[20] with additional fine tuning to optimize the performance of the PI control loop. Table 5 presents the parameters of the PI controllers.

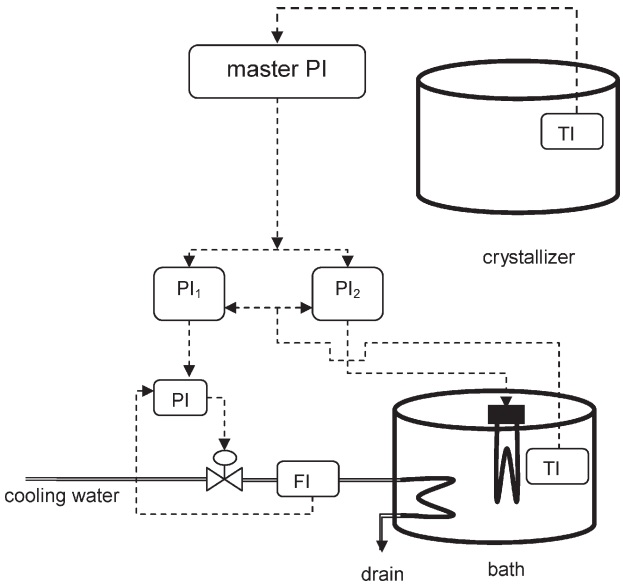
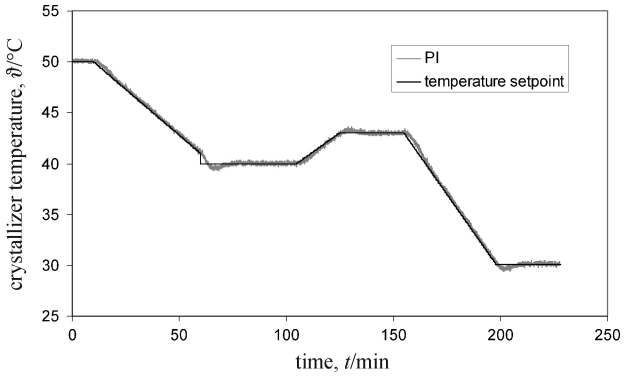


Fig. 8 – *PI configuration for crystallizer temperature control*

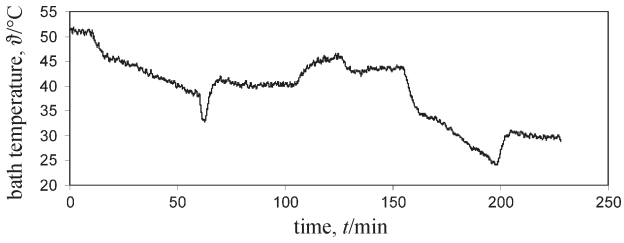
Table 5 – *Parameters of the PI controllers*

	K	t_I/s
PI_1	4	5
PI_2	79.58	40
master PI	5	230

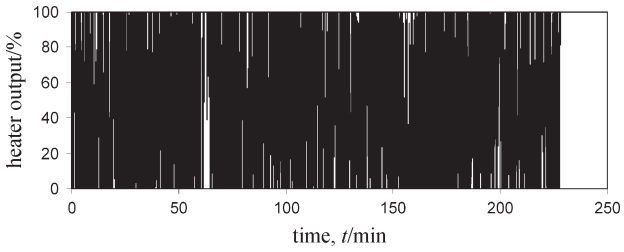
The performance of the PI control configuration has been tested by a series of step changes and ramps in the setpoint of the crystallizer temperature. The results of the setpoint tracking test of the PI configuration is shown in Fig. 9. The control actions of the PI control configuration for the crystallizer temperature control loop are shown in Figs. 10, 11 and 12.



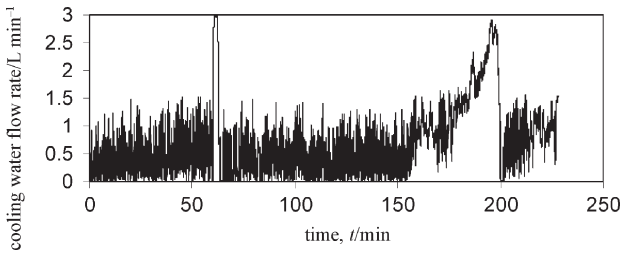
F i g . 9 – *Setpoint tracking test of the PI control configuration used in crystallizer temperature control loop*



F i g . 1 0 – *Water bath temperature in setpoint tracking test of the PI control configuration used in crystallizer temperature control loop*



F i g . 1 1 – *Heater duty in setpoint tracking test of the PI control configuration used in crystallizer temperature control loop*



F i g . 1 2 – *Cooling water flow rate in setpoint tracking test of the PI control configuration used in crystallizer temperature control*

Discussion

Although the crystallizer temperature has a large process delay (dead time) and a large process time constant, the DMC tracks the setpoint very well. The DMC predicts the future step changes and ramp changes and tries to eliminate the future errors as can be seen in Figs. 4 and 5. The effect of DMC prediction can be seen at times 10, 50, 100, 150 and 200 min. On the other hand, the PI controller responds to the changes after they have happened and does provide lower quality control of process with large dead time and time constant as seen in Figs. 9 and 10 at process times of 10, 50, 100, 150 and 200 min.

In addition to the setpoint tracking performance of the controllers, the controller manipulated changes can also be used to evaluate the controllers' performance. Figs. 6 and 11 show the heater changes of the DMC and PI configurations, respectively while Figs. 7 and 12 show the cooling water flow rate changes for DMC and PI controllers, respectively. It can be seen that the PI controller requires more aggressive changes in manipulated variables than that of the DMC. The DMC's optimizer provides optimum changes in the manipulated variables and the predictive nature of the DMC allows it to predict the future changes in the setpoint, thus mitigating sudden changes in the manipulated variables.

Conclusion

In this study, both DMC and PI controller configurations have been implemented on a mini pilot plant crystallizer unit. The dynamic behaviour of the water bath required two-step change models to represent the response of the water bath temperature to a step change in the water bath electrical heater duty and to the cooling water flow rate. In addition, one-step response model represents the temperature response of the crystallizer to a step change in the water bath temperature setpoint.

One slave SIMO DMC has been configured to control the water bath temperature. It captures the dynamics of the water bath using the step change models and manipulates the water bath electrical heater duty and the cooling water flow rate. In addition, one master SISO DMC controls the crystallizer vessel temperature by manipulating the setpoint of the water bath temperature control loop.

The performance of the DMC configuration has been compared to that of a PI controller configuration. The DMC performance resulted in a lower ISE and smaller overshoots than the PI controller which of course is due to the predictive nature of the DMC, in which the DMC by its very nature anticipates the future errors and reacts in such a way as to eliminate the future errors before they happen which is very effective for processes with relatively large time delays.

By comparing the control action of the DMC and PI controllers it can be seen that the PI controllers do result in a more aggressive control action than the DMC. The smoother control action of the DMC is due to the optimization procedure in the algorithm which prevents aggressive movements of the manipulated variables.

Nomenclature

DMC – dynamic matrix control
$\hat{E}$ – a $P \times 1$ vector which represents the error between the predicted values and the reference trajectory P sample time into the future
ISE – integral of square error
J – objective function
K – proportional gain of a PI controller
K_C – a $2M \times P$ matrix
M – control horizon
MPC – model predictive control
N – agitator speed, rev s^{-1}
N_i – number of coefficients of the step change model representing the effect manipulated variable i on the process variable
P – prediction horizon
PI – proportional-integral controller
Q – weighting matrix
R – weighting matrix
SIMO – single-input-multi-output
SISO – single-input-single-output
t_c – time constant, s
t_d – delay, s
t_I – integral time constant of a PI controller, s
ΔU – a $2M \times 1$ vector representing the M movements of manipulated variables
y – process variable
y_0 – initial value of the process variable

Greek letters

$\Delta u_i(\theta)$ – movement of the i-th manipulated variable at sample time θ
θ – sample time, s
ϑ – temperature, °C

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