Model Predictive Control of a Continuous Vacuum Crystalliser in an Industrial Environment: A Feasibility Study

N. Moldoványi[a,*] and J. Abonyi[b]

[a]Honeywell Process Solutions, Petneházy utca 2–4 Budapest, 1139-Hungary
[b]Department of Process Engineering, University of Pannonia, Egyetem utca 10 Veszprém, 8200-Hungary

Original scientific paper
Received: February 8, 2008
Accepted: November 5, 2008

Crystallisers are essentially multivariable systems with high interaction amongst the process variables. Model Predictive Controllers (MPC) can handle such highly interacting multivariable systems efficiently due to their coordinated approach.

In the absence of a real continuous crystalliser, a detailed momentum-model was applied using the process simulator in Simulink.

This process has been controlled by a model predictive controller widely used in industry. A new framework has been worked out for the incorporation of the Honeywell Profit® Suite controller to the simulator of the crystalliser. The engineering model and the controller were connected via OPC (OLE-Object Linking and Embedding for Process Control standard). Models were developed in Profit® Suite using the new fully-automated identification method. The feasibility study illustrated that the applied identification tool gave an accurate and robust model, and that the non-linear crystalliser may be controlled and optimised very well with the Honeywell Profit® Suite package. The developed system is proven to be useful in research and development.

Key words:
Model Predictive Control, feasibility study, continuous crystalliser, automated identification, OPC

Introduction

Crystallisation is a widely used cleaning, separation and grain-producing technique in the chemical industry, particularly within the pharmaceutical industries. The main quality criteria (from the point of view of controlling a crystalliser) are the properties of the produced crystals, that can be characterized based on the size-distribution of the crystals. Crystallisation is a multi-variable system with multi-input and multi-output (MIMO), often with strong coupling. Thus a good, modern approach to control is possible using a model-based MIMO control system. There are only a few examples in the literature for this.[1–5] A predictive type of control would be better than the corrective (feedback) type, because crystal size cannot be decreased under crystallisation conditions. One of the main problems is that (because of the mentioned properties of the population balance equation), for a proper model-based control of this size-distribution, a high-order control solution is required, which leads to technical difficulties.

Shi *et al.*[6,7] design predictive controllers for particle size distribution control (PSD), where the shape of the PSD is controlled by setting appropriate constraints on the shape of the PSD in the optimization problem that the predictive controller solves.

For the synthesis of the model based control system of the crystallisers, the momentum-model – generated from population balance equations as linear differential equations– can be used with close approximation. Chiu and Christofides[8] applied this property to design a non-linear single input single output (SISO) controller.

In this paper, a model predictive MIMO control system of a crystalliser is presented.

The crystalliser is connected to the controller using the OPC standard, which is the first step in applying model predictive controller for continuous vacuum crystallisers in the industry, and for simulators presented in published papers.[1–5]

For the synthesis of the control system, instead of a real continuous crystalliser, a moment model of the vacuum crystalliser was composed (Section 2, Appendix). The control problem (Section 3) and the applied, model predictive controller (Section 4) was presented. The linear model matrix for the model predictive controller was identified with a new fully-automated method in Honeywell Profit® Suite (Section 5). For the simulation the detailed model and the MPC of Honeywell, the Profit® Controller

*Corresponding author: nora.moldovanyi@honeywell.com

was connected via OPC; the simulation results (which gave very satisfactory results) are presented in Section 6. Comparison to PID controllers is shown in Section 7.

Mathematical model of a vacuum crystalliser

Consider a continuous MSMPR (mixed suspension mixed product removal) crystalliser in which supersaturation is generated using a vacuum. In this case, the crystalliser is considered as a three-phase operational unit; having liquid, solid and vapour phases, in which, under usual conditions, only two chemical species, the solvent and solute, take part in the crystallization process. (see Fig. 1) Then, the set of process level equations, termed rigorous model of the crystalliser, consists of the following balance equations:

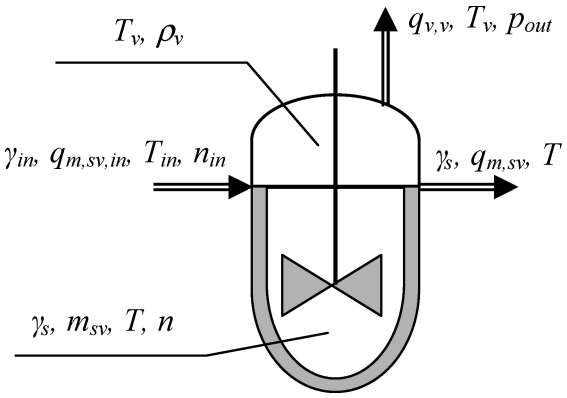


Fig. 1 – *Schematic of a vacuum crystalliser*

– Population balance equation for crystals governing the crystal size dynamics

– Mass balance equation for the crystallizing substance

– Mass balance equation for the solvent

– Energy balance equation for the vapour phase

It is assumed that the following conditions are satisfied:

(1) The volumetric feed and withdrawal rates of the crystalliser are constant and equal, thus the working volume is constant during the course of the operation;

(2) The crystals can be charaterised by a linear dimension L;

(3) All new crystals are formed at a nominal size $L_n \cong 0$ so that one can assume $L_n = 0$;

(4) Crystal breakage and agglomeration are negligible;

(5) No growth rate fluctuations occur;

(6) The overall linear growth rate of crystals G is size-dependent and has the form of the power law expression of supersaturation

$$G = \gamma(\gamma_{w,c}, \gamma_{w,e})\,\phi(L) = k_g(\gamma_{w,c} - \gamma_{w,e})^g\,\phi(L); \quad (1)$$

(7) The primary nucleation rate B_p is described by Volmer's model derived from the Gibbs-Thomson relationship:[9]

$$B_p = k_p \exp\left(-\frac{k_e}{\ln^2\left(\frac{\gamma_{w,c}}{\gamma_{w,e}}\right)}\right)\delta(L-L_n) = \beta_p\,\delta(L-L_n) \quad (2)$$

the secondary nucleation rate B_b is the following:

$$B_b = k_b(\gamma_{w,c} - \gamma_{w,e})^b\,\mu_3^j\,\delta(L-L_n) = \beta_b\,\delta(L-L_n) \quad (3)$$

Where:

$$k_g = k_{g0}\exp\left(-\frac{E_g}{RT}\right);\ \ldots\ k_p = k_{p0}\exp\left(-\frac{E_p}{RT}\right);$$
$$k_b = k_{b0}\exp\left(-\frac{E_b}{RT}\right) \quad (4)$$

where μ_3 is the third of the ordinary moments of the population density function n, which are defined as:

$$\mu_m = \int_0^\infty L^m n(L,t)\,\mathrm{d}L, \qquad m = 0,1,2,3\ldots \quad (5)$$

The modelled variables are: μ_0, μ_1, μ_2, μ_3, w_c, m_{sv}, T, ρ_v, T_v, i.e. the zero, first, second and third order moments of the crystal size, concentration of the solute, the solvent mass, the temperature of suspension, the vapour density and the temperature of vapour, respectively. The final moment equation model is summarised in the Appendix; the details can be found in the paper of Ulbert and Lakatos.[10]

The control problem

The goal of the above presented crystalliser is to produce crystals with a certain quality as far as possible using the minimum amount of energy. From the point of view of controlling a crystalliser the main quality criteria are the properties of the produced crystals, the size and the size-distribution. The quantity of the produced crystals, the delivery of the crystalliser can be also controlled. So, the

outputs, the variables to be controlled (called CVs), calculated from the moments are the following:

– Mean crystal size, calculated from the moments $\mu_1/\mu_0 = (x_1/S_1)/(x_2/S_2)$

– Standard deviation of the crystal size distribution computed as:

$\sigma^2 = \mu_2/\mu_0 - (\mu_1/\mu_0)^2 = (x_2/S_2)/(x_0/S_0) - ((x_1/S_1)/(x_0/S_0))$

– μ_3, delivery of the crystalliser, where $k_V \mu_3$ is the volume of the produced crystals

Where $S_{T,t,0,1,2}$ are dimensionless parameters, $x_{0,1,2}$ are the dimensionless moments.

From the process point of view, in a continuous vacuum crystalliser, the pressure, the temperature and the residence time can be changed in practice. In the environment of the model the inputs, the variables to be manipulated (called MVs), are the following:

– Pressure; can be changed with partial pressure, by the valve constant K_s of the vapour outlet

– Temperature; can be changed with x_{7in} dimensionless inlet suspension temperature, where $x_{7in} = T_{sus,\ in}\ S_T$

– Residence time; can be varied with ξ_{av} dimensionless residence time, where $\xi_{av} = \tau_{mean}\ S_t$

There is a strong coupling between the inputs and the outputs, for example by changing the residence time in the vacuum crystalliser not only the size but the size distribution (and of course the delivery) changes.

Since its proposal by Bristol in 1966,[11] the relative gain technique has not only become a valuable tool for the selection of manipulative-controlled variable pairings, it has also been used to predict the behaviour of controlled responses. The relative gain array (RGA) can be easily calculated from the gains of the model matrix presented below (K):

$$\mathbf{\Lambda} = \mathbf{K} \cdot (\mathbf{K}^T)^{-1} \tag{6}$$

$$\mathbf{\Lambda} = \begin{bmatrix} 0 & 2.651 & -1.651 \\ 0.837 & -2.669 & 2.832 \\ 0.163 & 1.018 & -0.181 \end{bmatrix} \tag{7}$$

It is an obvious proof of strong coupling.

To summarise, the above presented crystalliser is a non-linear object, with a high degree of interaction between the process variables. One can do nothing if the crystals grow beyond a certain size. For all of these problems, a model predictive controller presents a good solution. MPC can handle the MIMO object; and it is predictive, so the controller "prevents" over-size crystals. In Section 7 a comparison to PID controllers is presented. For non-linearity within a certain range, a robust controller is adequate as the results presented below show. The integration of a process simulator and the MPC of Honeywell was performed with OPC (originally OLE-Object Linking and Embedding for Process Control).[12] This standard specifies the communication of real-time plant data between control devices from different manufacturers. OPC was designed to bridge Windows-based applications and process control hardware and software applications.

Model predictive control

Model predictive control (MPC) refers to a class of computer control algorithms that utilise an explicit process model to predict the future response of the plant.[13] Originally developed to meet the specialised control needs of power plants and petroleum refineries,[14] MPC technology can now be found in a wide variety of application areas including chemicals, food processing, automotive and aerospace applications. The presented work is an opening to another new application, the MPC control of continuous crystallisers.

In model predictive control the control action is provided after solving – on-line at each sampling instant – an optimisation problem, and the first element in the optimised control sequence is applied to the process (receding horizon control). The "moving horizon" concept of MPC is a key feature that distinguishes it from classical controllers, where a pre-computed control law is employed. A major factor in the success of model based predictive control is its' applicability to problems where analytical control laws are difficult, or even impossible to obtain.

A model is used to predict the future plant outputs, based on past and current values and on the proposed optimal future control actions. These actions are calculated by the optimiser, taking into account the cost function (where the future tracking error is considered) as well as the constraints. The methodology of all the controllers belonging to the MPC family is characterised by the following strategy, represented in Fig. 2 (u is the input y is the output and w is the set-point). From the Section 3 with this classical notation $\boldsymbol{u} = (K_s, x_{7in}, \xi_{av})$, and the $\boldsymbol{y} = (\mu_1/\mu_0, \sigma^2, \mu_3)$. Controllability test has been also performed and even the subspace of the operating region was defined.[15]

For MPC the prediction horizon (H_p) represents the number of samples taken from the future over which MPC computes the predicted process variable profile and minimises the predicted error. The control signals change only inside the control horizon, H_c remaining constant afterwards:

$$u(k+j) = u(k+H_c-1), \quad j = H_c, \ldots, H_p - 1$$

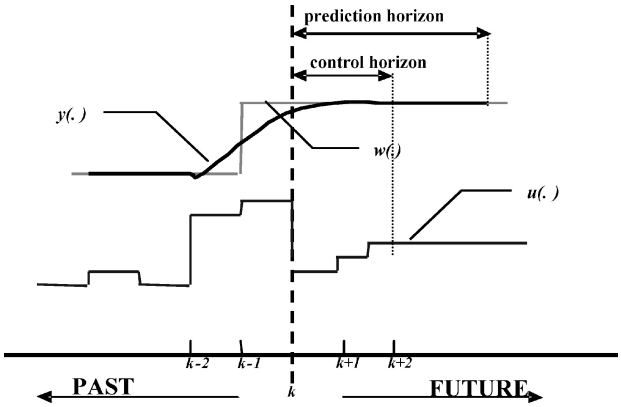


Fig. 2 – *MPC horizons*

The basic steps:

1. In the MPC future outputs for a determined prediction horizon H_p are predicted at each instant k using a prediction model. These predicted outputs $\hat{y}(k+j|k)$, $j=1,\ldots H_p$ (means the value at the instant $k+j$, calculated at instant k) depend on the known values up to instant k (past inputs and outputs) and the future control signals $u(k+j|k)$, $j=0,\ldots H_p-1$, which are those to be sent to the system and to be calculated.

2. The set of control signals is calculated by optimising a cost function in order to keep the process as close as possible to the reference trajectory $w(k+j)$, $j=1,\ldots H_p$ or to keep inside the range.

3. The control signal $u(k|k)$ is sent to the process whilst the next control signals calculated are rejected, because at the next sampling instant $y(k+1)$ is already known and step 1 is repeated with this new value and all the sequences are updated. Thus the $u(k+1|k+1)$ is calculated (which in principle will be different to the $u(k+1|k)$ because of the new information available) using a receding horizon concept.

The details of MPC are presented by Moldoványi and Lakatos.[16]

Honeywell's Profit® Controller controls the process using the minimum manipulated variable movement necessary to bring all of the process variables within limits or to setpoints; and to optimise the process with the remaining degrees of freedom in order to drive the process to optimum operation. Profit Controller uses the Honeywell patented Range Control Algorithm (RCA).[17] RCA minimises the effects of model uncertainty while determining the smallest process moves required to simultaneously meet control and optimisation objectives. The robustness of the controller is tested in this study, since a non-linear object was controlled with a linear MPC. The issues of using a linear controller in order to control a non-linear process may not be as big an issue as is first expected. There are two reasons for this. Firstly, the non-linearity, non-linear region or non-linear variable(s) may sometimes be linearised where it is well understood. Secondly, within the relatively narrow range of normal operation of a process, the process may be said to act linearly within these limits.

Profit® Controller application includes the necessary tools to design, implement and maintain MIMO applications. In the next section a new release of the off-line model identifier, the practical global multi-stage method for fully automated identification is presented.

Identification of the models

For a good model predictive control, a good model and a robust controller is needed (robustness being the ability to cope with model error). In the following section, the applied automated identification of Honeywell is presented.

The basic idea of the new fully automated identification[18] is that no single method is adequate for the range of conditions encountered in the target industries. Hence, this approach utilises a family of prediction error model derived structures and consequently a family of model orders for each structure. These families are then searched for the most effective model for the given application.

For a given set of data only one identification pass is required. The approach was designed to work equally well under both open and/or closed-loop conditions. As this approach is a multi-stage, multi-structure method, many different model structures may be returned as a solution. Any model resulting from these calculations is designated as a "CLid" model in Honeywell.[17] The identification has been done offline. The identification data has been collected in open-loop tests.

Any empirical based technique would give some indication as to the quality of the computed results. Identification is no exception. To be practical, model quality should be unambiguous. This implies that the information must not only indicate the "goodness" or lack of fit, but also indicate the validity of the model. This point is often ignored but is critical in practical applications since in most cases causal relationships between each input and output do not exist.

The basic sequential is the following:

1. Precondition data

– Scale and remove means from discontinuous data segments

2. Calculate tentative time delay for all channels

– Establish time delay for the range of expected orders

3. Calculate candidate model sets for each structure for each order

– Calculate high order model for initial conditions (IC) of all models requiring an iterative search

– Reduce IC model order prior to search

– Estimate model parameters both with and without the tentative time delay. Select parameters that result in a minimum loss function

– Reduce model order

– Establish first instance of model quality independent of predictive performance

– Rank each input-output model pair based on quality metric

4. Design band pass filter based on current model set

– One filter for special band pass model

– One filter for predictive metric

5. Generate model set based on band pass filtered data

6. Generate predictive metrics for all model sets on transformed data

7. Update model quality and ranking based on predictive metric

8. Perform global search using combined model quality and predictive metric as a performance measure

9. Reduce model order where possible

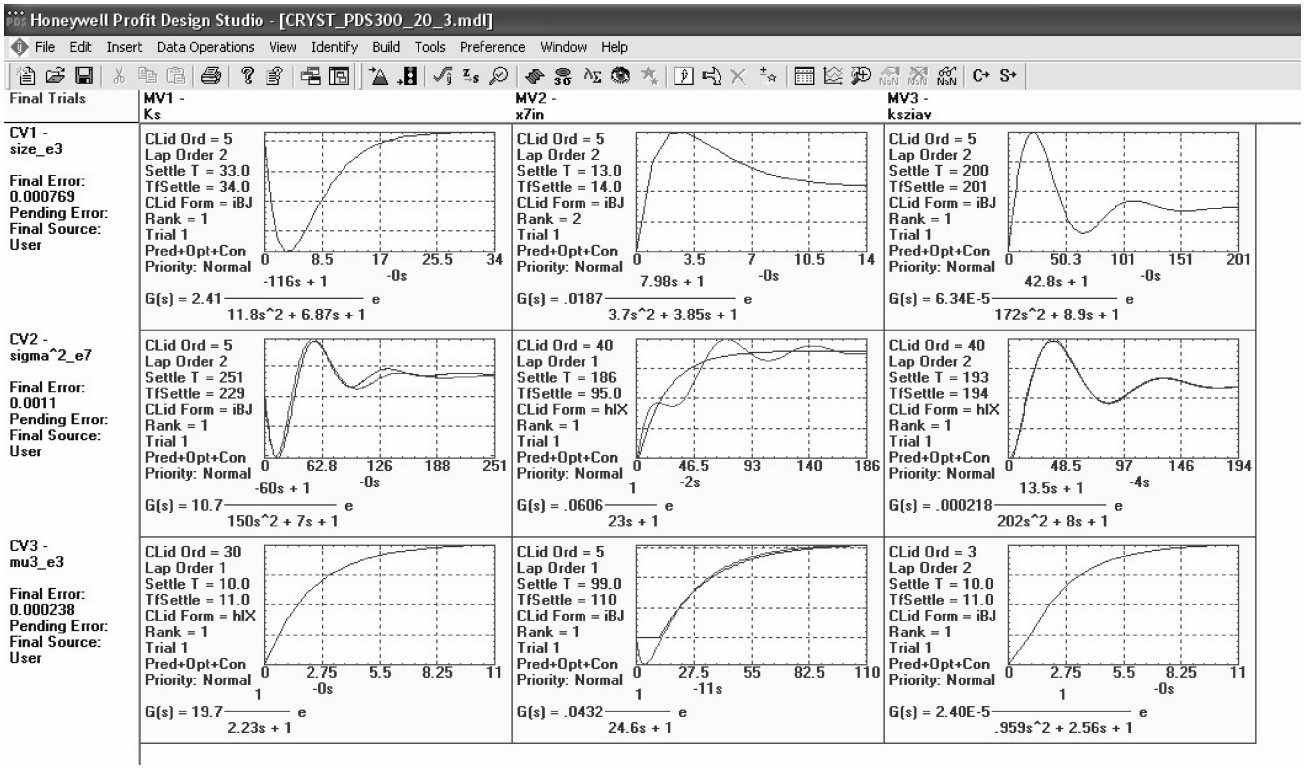
10. Update model metrics for final reduced order model

Instead of a real unit, the model of the crystalliser – presented above – was excited by steps in Matlab Simulink environment to collect data for the identification of the model matrix. Profit® Controller uses a model to predict process behaviour. The overall process model is composed of a matrix of dynamic sub-process models, each of which describes the effect of one of the independent variables on one of the controlled variables. A sub-process model describes how the effect of an independent variable on a control variable evolves over time. It is called the matrix of linear dynamic sub-process models, the linear model matrix.

Each manipulated variable (pressure, temperature, residue time) was stepped many times one by one considering the time to steady state, as would be carried out in an industrial project environment. The process was stepped around a stable operating point with reasonable step sizes as tested before.

With the collected data the above presented automated method was use for the model identification in Profit® Design Studio.

The identification result is shown in Fig. 3. The manipulated variables (MV1 = K_s, MV2 = x_{7in}, MV3 = ξ_{av}), are in columns, the controlled variables (CV1 = μ_1/μ_0, CV2 = σ^2, CV3 = μ_3) are in the rows. For better conditioning of the problem, the magni-



F i g . 3 – *Model matrix of the vacuum crystalliser, identified in Profit® Design Studio (The lighter line is the data from the step test, the darker line is the modelled function)*

tudes of the CVs were changed; multiplied by 10^3, 10^7, 10^3 respectively. The model is the darker line, the data is the lighter, often covered.

Profit® Design Studio found good models quickly with the automated identification method.

In this case the model matrix is full, all the CVs are in connection to all the MVs, as we saw at the RGA, eq. (7). With pressure (MV1), the size (CV1) and the size-distribution (CV2) models have a highly inverse response, by increasing the pressure, the size and size-distribution decreases first and then increases, because the nucleation is changing. With this accurate identification the high order sub-models can follow the special behaviour of the object.

The inlet temperature (MV2) – delivery (CV3) model also appears to be an inverse response model, because by increasing the temperature, the discharge temporary increased. But it was simplified to deadtime, because it could "mislead" the optimiser, the temperature has to be increased to maximise the delivery. In any case, the inverse response is not inverted by Profit Controller but is treated as deadtime from a control point of view, so simplifying it to deadtime makes little difference to the control algorithm results although "real" inverse response can improve predictions a little. Removing inverse response models can be a matter of engineering judgement.

The temperature (MV2) – size-distribution (CV2) model was simplified, a first order model is good enough to model this dynamic. The MV1-CV2 model was also simplified. The residue time (MV3) models with size (CV1) and size-distribution (CV2) have much bigger overshoots, than MV2-CV2 model, so these models were not simplified from the high order models.

Control study

In the absence of a real crystalliser, the engineering model acts like the unit, connected to the controller via OPC. For the non-linear model in Matlab the inputs are the MVs, which are the controller outputs. The Matlab model calculates the CVs and sends them to the controller via OPC every minute, see Fig. 4.

The control horizon (where the manipulated variables changes in the prediction) contains 10 movements of the MVs in the Honeywell controller.

The prediction horizon (where the prediction is calculated) is the closed loop response interval, this is about 1.5 hours in this case. This value should be calculated based on the knowledge of the system dynamics. Hence, in case of Honeywell Profit Controller this value has been calculated from the models automatically.

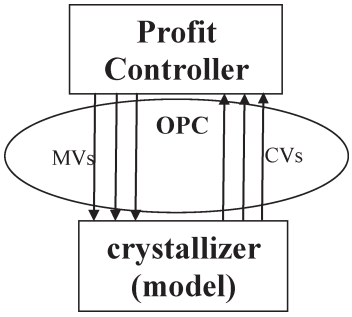


Fig. 4 – *The control scheme with Profit Controller*

Weights of MVs, rate of change limits and ramping limits, and other tuning parameters were set up in Profit Controller.

The size was controlled to a setpoint, it followed the changes that were made correctly. The cost function, which the optimizer is trying to minimize – if there is a degree of freedom for it – is $J = \sigma^2 - 10\mu_3$; it means that the standard deviation of the size distribution was minimised within a range, but the maximisation of the volume was set to be a more important priority

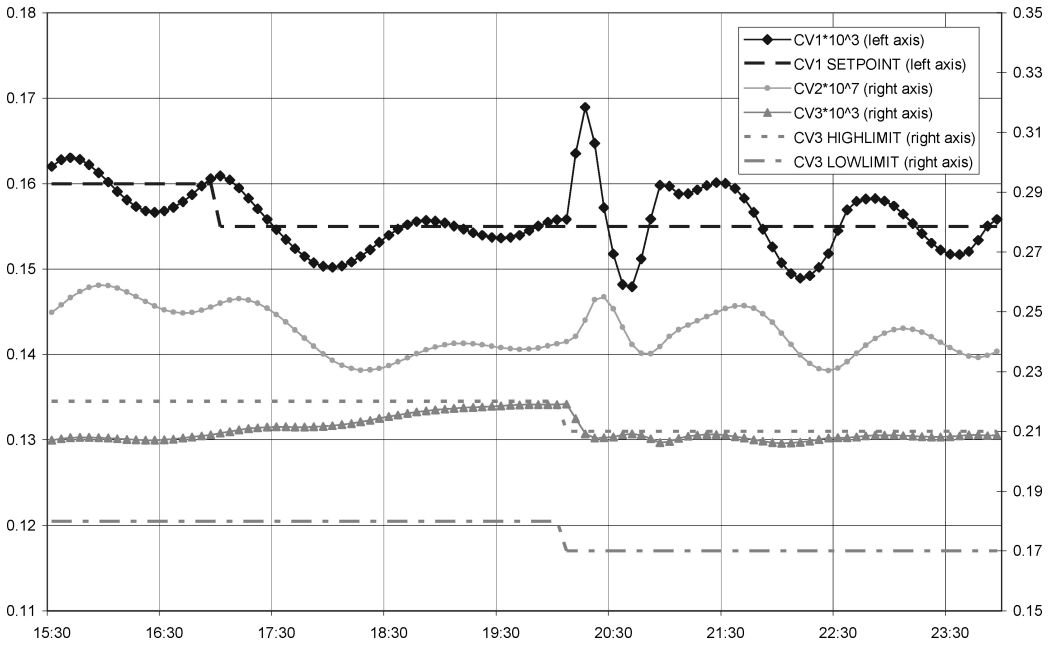
The optimisation speed factor is 5 (fast), which results in an optimisation horizon approximately 6/5 times the CV overall response time. The CV overall response time is defined as the average of the longest CV response time and the average CV response time, 123 min in this case.

The simulation results are shown in Fig. 5a and b. The dashed lines are the setpoint for CV1 and the minimum and the maximum limits of CV3. The limits of CV2 are irrelevant.

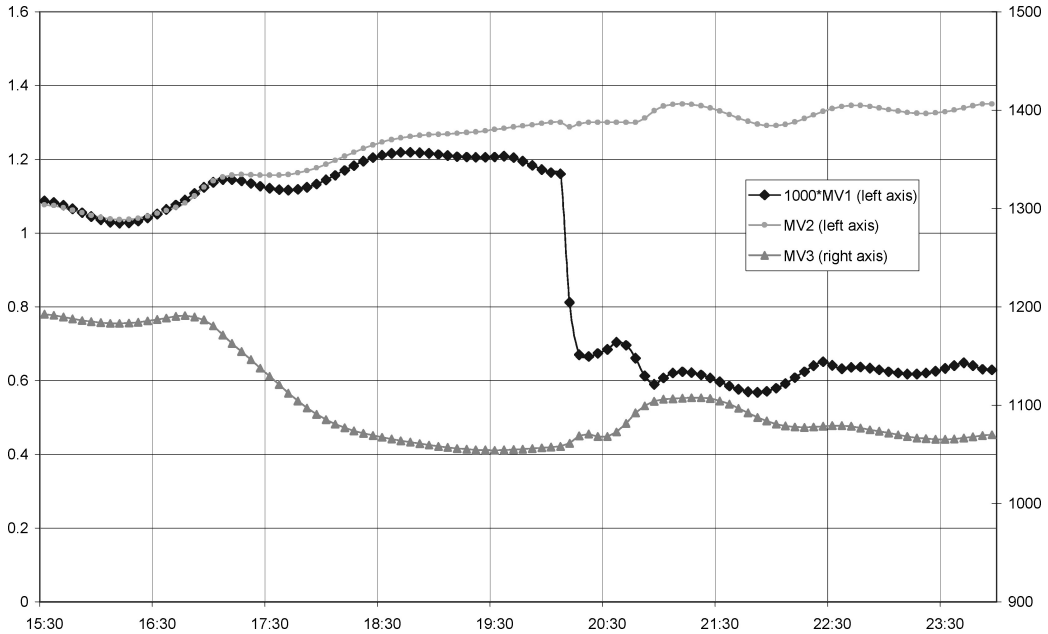
In the test run the optimiser was turned on at 16:40, from that time the CV3 (delivery) increased significantly, the CV2 (size distribution) decreased a little to the optimal values. CV1 setpoint change is solved after a little overshoot, the changes of MVs (Fig. 5b) show that the controller reacts rapidly. When the range of CV3 is changed, the MVs change fast, and the control problem is solved. CV1 also changed significantly due to interaction, but it calms down after a while.

The results show that the controller optimises and solves the changes in the range, the MVs react rapidly, but smoothly, and the controller is robust.

The online measurement of size distribution can be complicated. With Profit Controller the size distribution can be an inferred variable, calculated from measurable variables and updated from measurement. It is an often-used technology, for example to control the cutpoints in the refineries. Therefore, the applicability of the proposed control



F i g . 5 a – *Simulation results for the MPC controller, optimiser, with controlled variables (CV1 = crystal size, CV2 = crystal size-distribution, CV3 = delivery of the crystalliser)*



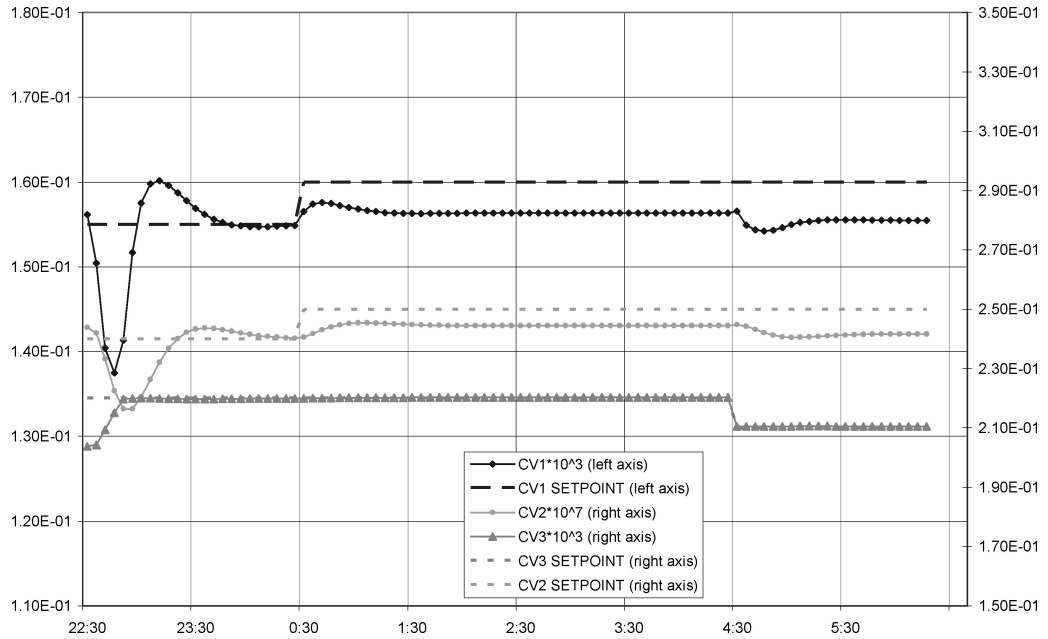
F i g . 5 b – *Simulation results for the MPC controller, optimiser, with manipulated variables (MV1 = pressure, MV2 = temperature, MV3 = residence time)*

schema in industrial environment requires the applicability of online measurement system or the development of advanced soft sensor based state estimation algorithms.

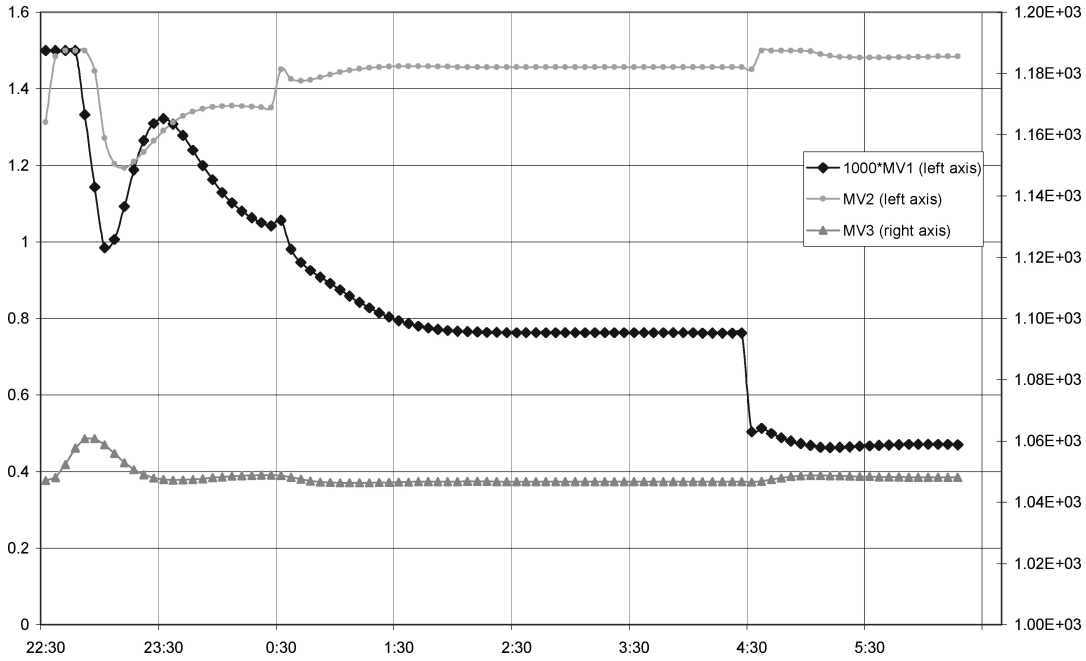
Comparison with PID controllers

To compare the advanced, model predictive controller results, basic level, PID controllers were set up and tuned for the vacuum crystalliser.

One main advantage the MPC to the set of PIDs is that the structural problems are solved inherently, MPC handles the assigning loops. There is a difference in complexity between the two controllers. According to engineering experience the more complex the technology the more complex the control system, but the slope of the relation depends on the kind of controller. For simple cases, PID is easier, but for a difficult one MPC can be the easier controller to implement. Already for this 3 input, 3 output case the decoupling is difficult, MPC can handle the MIMO object without problem.



F i g . 6 a – *Simulation results for the PID controllers, with controlled variables (CV1 = crystal size, CV2 = crystal size-distribution, CV3 = delivery of the crystalliser)*



F i g . 6 b – *Simulation results for the PID controllers, with manipulated variables (MV1 = pressure, MV2 = temperature, MV3 = residence time)*

PID is a single input single output (SISO) controller and as it is shown in the control studies, the crystallisers are MIMO object with strong coupling. According to eq. (7) the only solution is that MV1 controls CV3, MV2 controls CV1 and CV2 is controlled by MV3.

$$\mathbf{\Lambda} = \begin{bmatrix} 0 & \mathbf{2.651} & -1.651 \\ 0.837 & -2.669 & \mathbf{2.832} \\ \mathbf{0.163} & 1.018 & -0.181 \end{bmatrix} \qquad (8)$$

The starting points of the PID tunings were calculated with the strategy based on Internal Model Control (IMC). The parameters of the PID controllers were fine-tuned.

In the simulation run the setpoints are the same like the steady state values were in the study of MPC. The result (Fig. 6a and b) shows that the coupling is strong, PID controllers can not really handle this MIMO object. The new

setpoint of CV1 couldn't reach, but for CV3 it is good.

It is clearly shown that MPC can control the crystalliser better, but to compare the simulation results with a number in a simple way, G average deviation was calculated from the time of the change of the setpoint of the first controlled variable:

$$G = \frac{\sum_{\text{steptime}}^{\text{steptime}+3\text{ h}} (\text{CV1} - \text{CV1\_setpoint})^2}{\text{number of samples}} \quad (9)$$

– MPC with the high order models $G = 7.02 \cdot 10^{-6}$

– MPC with the simplified models $G = 4.85 \cdot 10^{-6}$

– PID controllers $G = 1.23 \cdot 10^{-5}$

The difference of the MPCs with high and low order models would be bigger with real model errors.

With the PID controllers the new setpoint was not really reached. The reason can be that the operating points coming from the MPC simulation study are unreachable with PIDs or the tuning can be the problem.

Conclusion

Crystallisers are multivariable objects with coupling among the process variables. Model predictive controllers (MPC) can handle such highly interacting multivariable systems.

In the absence of a real continuous crystalliser, a detailed moment model was applied. The engineering model and the controller were connected via OPC.

The model predictive control study was performed in the Honeywell Profit® Suite environment, using the new fully automated identification method. The results show that the identification is accurate, the non-linear object was controlled and optimised very well with Honeywell's MPC, Profit Controller. The controller is robust.

Comparing different types of controllers, the results also illustrate that MPC can solve the control problem much better that PID.

ACKNOWLEDGEMENTS

Special thanks to Professor Bela Lakatos from the University of Pannonia and colleagues at Honeywell, Howard Boder and Peter Kiss for their good ideas and review.

Appendix

The moment equation model of a continuous vacuum crystalliser is formed by the following equations.[10]

Zero order moment:

$$\frac{\mathrm{d}\mu_0}{\mathrm{d}t} = \frac{q_{m,sv,in}}{m_{sv}}(\mu_{0,in} - \mu_0) + B + \frac{\mu_0}{m_{sv}}W_v, \quad B = B_p + B_b \quad (A1)$$

First order moment:

$$\frac{\mathrm{d}\mu_1}{\mathrm{d}t} = \frac{q_{m,sv,in}}{m_{sv}}(\mu_{1,in} - \mu_1) + \gamma(\gamma_{w,c}, \gamma_{w,e})(\mu_0 + a\mu_1) + \frac{\mu_1}{m_{sv}}W_v \quad (A2)$$

Second order moment:

$$\frac{\mathrm{d}\mu_2}{\mathrm{d}t} = \frac{q_{m,sv,in}}{m_{sv}}(\mu_{2,in} - \mu_2) + \gamma(\gamma_{w,c}, \gamma_{w,e})(\mu_1 + a\mu_2) + \frac{\mu_2}{m_{sv}}W_v \quad (A3)$$

Third order moment

$$\frac{\mathrm{d}\mu_3}{\mathrm{d}t} = \frac{q_{m,sv,in}}{m_{sv}}(\mu_{3,in} - \mu_3) + \gamma(\gamma_{w,c}, \gamma_{w,e})(\mu_2 + a\mu_3) + \frac{\mu_3}{m_{sv}}W_v \quad (A4)$$

Mass balance for solute:

$$\frac{\mathrm{d}\gamma_{w,c}}{\mathrm{d}t} = \frac{q_{m,sv,in}}{m_{sv}}(\gamma_{w,c,in} - \gamma_{w,c}) - 3k_V\rho\gamma(\gamma_{w,c} - \gamma_{eq})(\mu_2 + a\mu_3) + \frac{\gamma_s}{m_{sv}}W_v, \quad (A5)$$

Mass balance for the solvent:

$$\frac{\mathrm{d}m_{sv}}{\mathrm{d}t} = q_{m,svin} - q_{m,sv} - W_v \quad (A6)$$

Energy balance equation for the crystal suspension:

$$\frac{\mathrm{d}T}{\mathrm{d}t} = \frac{q_{m,sv,in}}{C_{av}m_{sv}}C_{av,in}(T_{in} - T) - \Delta h_v\frac{W_v}{C_{av}m_{sv}} + 3k_V\rho\gamma(\gamma_s - \gamma_{eq})(\mu_2 + a\mu_3)\frac{\Delta h_c}{C_{av}} \quad (A7)$$

where

$$C_{av} = C_{sv} + C_c + k_V\rho C\mu_3$$

and

, $$C_{av,in} = C_{sv} + C_{c,in} + k_V\rho C\mu_{3,in}.$$

Mass balance equation for the vapour phase:

$$\frac{\mathrm{d}\rho_v}{\mathrm{d}t} = \frac{1}{V_v}\left[\left(1 - \frac{\rho_v}{\rho_{sv}}\right)W_v - \rho_v q_{v,v} + \rho_v q_{m,sv,in}\left(\frac{1}{\rho_{sv}} + \frac{y_{in}}{\rho} + k_V\mu_{3in}\right) - \rho_v q_{m,sv}\left(\frac{1}{\rho_{sv}} + \frac{y}{\rho} + k_V\mu_3\right)\right] \quad (A8)$$

where the steam removal of the evaporated solvent was modelled by a control valve having characteristics

$$q_{m,v} = \rho_v q_{v,v} = \rho_v K_s\sqrt{p_v(p_v - p_{out})}. \quad (A9)$$

Energy balance equation for the vapour phase:

$$\frac{\mathrm{d}T_v}{\mathrm{d}t} = -\frac{C_v(T_v - T)W_v}{V_v\rho_v\left(C_v + (T_v - T)\frac{\mathrm{d}C_v}{\mathrm{d}T_v}\right)}. \quad (A10)$$

Where:

$$V_v = V - m_{sv}\left(\frac{1}{\rho_{sv}} + \frac{y}{\rho} + k_v\mu_3\right) \quad \text{(A11)}$$

The constitutive equations associated with the moment, mass and energy balance equations were as follows.

Temperature dependence of the solubility:

$$\gamma_s(T) = a_0 + a_1T + a_2T^2 \quad \text{(A12)}$$

Evaporation rate of the solvent:

$$W_v = K_{evap}(p_v - p_v^*) \quad \text{(A13)}$$

where the vapour pressure was computed by the Antoine-equation:

$$\log p_v^* = A_A - \frac{B_A}{T + C_A} \quad \text{(A14)}$$

While the state of vapour was predicted by the ideal gas law:

$$p_v = \frac{m_v R T_v}{V_v}. \quad \text{(A15)}$$

List of symbols

APC – advanced process control
CV – controlled variable
DV – disturbance variable
MPC – model predictive controller
MV – manipulated variable
OPC – originally OLE for process control
OLE – object linking and embedding
RCA – range control algorithm
SS – steady state
a – constant of the crystal growth rate, m^{-1}
b – exponent of secondary nucleation rate
B_p – primary nucleation rate, m^{-3} s^{-1}
B_b – secondary nucleation rate, m^{-3} s^{-1}
C – heat capacity, J kg^{-1} K^{-1}
D_{ap} – dimensionless parameter for primary nucleation
D_{ab} – dimensionless parameter for secondary nucleation
g – exponent of crystal growth rate
G – crystal growth rate, m s^{-1}
h – specific enthalpy, J kg^{-1}
j – exponent of secondary nucleation rate
k_e – parameter of primary nucleation rate
k_g – rate coefficient of crystal growth, m^{3g+1} kg^{-g} s^{-1}
k_p – rate coefficient of primary nucleation, m^{-3} s^{-1}
k_b – rate coefficient of secondary nucleation, m^{3b-3} kg^{-b} s^{-1}
k_V – volume shape factor, m^3
K_s – constant, m^4 s kg^{-1}
K_{evap} – constant, m s
L – linear size of crystals, m
m – mass, kg
N – number of nucleus
n – population density function, m^{-4}
p – pressure, Pa
q_m – mass flow rate, kg s^{-1}
q_v – volumetric flow rate, m^3 s^{-1}
s_c – scale factor of the concentration, kg^{-1} m^3
s_m – scale factor of the m^{th} order moment of n (m = 0, 1, 2,…)
S_T – scale factor of the temperature, C^{-1}
S_t – scale factor of the time, s^{-1}
V – volume, m^3
x_m – m^{th} order dimensionless moment (m = 0, 1, 2,…)
y – dimensionless concentration of solute
W – evaporation rate, kg s^{-1}

Greek letters

α – dimensionless parameter
β – dimensionless parameter
γ – crystal growth rate, s^{-1}
γ_s – concentration of solute, kg m^{-3}
γ_{eq} – equilibrium saturation concentration, kg m^{-3}
δ – parameter of Volmer's model
ε – voidage of suspension
μ_m – m^{th} order moment of n, m^{m-3}
Θ – dimensionless nucleation rate
ρ_c – density of crystals, kg m^{-3}
ξ – dimensionless time
Φ – crystal size, m

Subscripts

0 – initial value
in – inlet value
p – primary nucleation
b – secondary nucleation
S – steady state
v – vapour

References

1. *Qin, S. J., Badgwell, T. A,* Control Engineering Practice **11** (2003) 733.
2. *Myerson, A. S., Rush, S., Schork, F. J., Johnson, J. L.,* Proc. 10th Symposium. Industrial Crystallization, Academia, Praha, 1987.
3. *Jager, J., Kramer, H. J. M., deJong, E. J., de Wolf, S., Bosgra, O. H., Boxman, A., Merkus, H. G., Scarlett, B.,* Powder Technology **69** (1992) 11.
4. *Miller, S. M., Rawlings, J. B*., AIChE Journal **40** (1994) 1312.
5. *Rohani, S., Haeri, M., Wood, H. C.,* Computers and Chemical Engineering **23** (1999) 279.
6. *Shi, D., El-Farra, N. H., Li, M., Mhaskar, P., Christofides, P. D.,* Chem. Eng. Sci. **61** (2006) 268.

7. *Shi, D., El-Farra, N. H., Li, M., Mhaskar, P., Christofides, P. D.,* Nanotechnology **16** (2005) S562.
8. *Chiu, T., Christofides, P. D.,* AIChE Journal **45** (1999) 1279.
9. *Mullin*, *J. W.,* Crystallization, Butter-Worth-Heinemann, Oxford, 1993.
10. *Ulbert, Zs., Lakatos, B. G.,* Simulation of CMSMPR vacuum crystallisers. Computers and Chemical Engineering **23** (1999) S435.
11. *Bristol, E. H.,* IEEE Trans. on Auto. Control AC-11 (1966) 133.
12. http://www.opcfoundation.org
13. *Meadows, E. S., Rawlings, J. B.,* Model predictive control, Chapter 5., Englewoods Cliffs. NJ, Prentice-Hall, 1997, pp. 233–310.
14. *Joe Qin, S., Badgwell, T. A.,* Control Engineering Practice **11** (2003) 733.
15. *Nora Moldovanyi,* PhD thesis, http://twilight.vein.hu/phd_dolgozatok
16. *Moldoványi, N., Lakatos, B. G.,* Hungarian Journal of Industrial Chemistry **33** (2005) 97.
17. R300 Profit Suite Documentation, Identifier User's Guide AP09-200, Honeywell International Inc., 2007
18. *MacArthur, J. W., Zhan, Ch.,* Journal of Process Control, in press doi:10.1016/j.jprocont. 2007.04.003