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CONTROL OF A CONTINUOUS VACUUM CRYSTALLISER IN AN INDUSTRIAL ENVIRONMENT: A FEASIBILITY STUDY – COMPARISION PID TO MODEL PREDICTIVE CONTROL SOLUTION

N. MOLDOVÁNYI[1], J. ABONYI[2]

[1]Honeywell Process Solutions, H-1139 Budapest Petneházy u. 2-4 HUNGARY,
[2]University of Pannonia, Department of Process Engineering, H-8201 Veszprém, P.O. Box 158, HUNGARY

Crystallisers are essentially multivariable systems with high interaction amongst the process variables, that's why it is a difficult control problem. In the absence of a real continuous crystalliser, a detailed momentum-model was applied using the process simulator in Matlab Simulink. The relative gain array was calculated to try to decouple the input and output variables for the setup of single input single output (SISO) PID controllers. The PIDs were tuned, but the control performance is not satisfying.

Model Predictive Controllers (MPC) can handle such highly interacting multivariable systems efficiently due to their coordinated approach. The feasibility study illustrated that the applied identification tool gave an accurate and robust model, and that the non-linear crystalliser can be controlled and optimised very well with the Honeywell Profit® Suite package. The developed system – engineering model in Matlab is connected to an MPC used in the industry via OPC (originally OLE-Object Linking and Embedding for Process Control) - is proven to be useful in research and development.

Keywords: Continuous crystalliser, feasibility study, model predictive control

Introduction

Crystallization 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—let us first consider size-distribution and size. 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 crystallization 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. The crystallisers are dissipative systems [6]; hence, a crystalliser as a dynamical system possesses finite-dimensional global attractors [7] that create an adequate basis for the synthesis and use of a good quality, low order model-based control system.

At the same time, it means that 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.

To select a proper controller structure first SISO PID controllers after a model predictive MIMO control systems of a crystalliser are presented in this paper. One main advantage the MPC to the set of PIDs is that the structural problems are solved inherently, MPC handles the assigning loops.

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 dynamic analysis of the model (Section 4) was presented. In Section 5 the crystalliser was tried to control with PID controllers. Another kind, more adequate controller, the model predictive controller is presented is Section 6. For the simulation the detailed model and the MPC of Honeywell, the Profit Controller was connected via OPC (originally OLE-Object Linking and Embedding for Process Control); the simulation results (which gave very satisfactory results) are presented in Section 7. In the end some comparison is made to PID controller and MPC.

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*.)

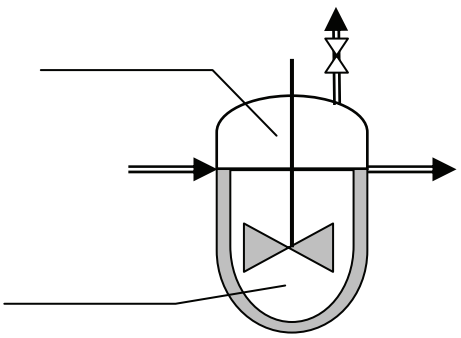

Figure 1: Schematic of a vacuum crystalliser

Then, the set of process level equations, termed rigorous model of the crystalliser, consists of the following balance equations:

- 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 characterized by a linear dimension L;

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

(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

$$G = \gamma(w_c, w_e)\phi(L) = k_g\left(w_c - w_e\right)^g \phi(L); \qquad (1)$$

(7) The primary nucleation rate B_p is described by Volmer's model:

$$B_p = k_p \exp\left(-\frac{k_e}{\ln^2\left(\frac{w_c}{w_e}\right)}\right)\delta(L - L_n) = \beta_p\delta(L - L_n) \qquad (2)$$

the secondary nucleation rate B_b is the following:

$$B_b = k_b\left(w_c - w_{ce}\right)^b \mu_3^j \delta(L - L_n) = \beta_b\delta(L - L_n) \qquad (3)$$

where:

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

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

$$\mu_m = \int_0^\infty L^m n(L,t)dL, \qquad m = 0,1,2,3... \qquad (5)$$

The model variables are: μ_0, μ_1, μ_2, μ_3, W_C, M_{SV}, T, P_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 [9].

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 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, S_t, S_0, S_1, S_2 are dimensionless parameters, x_0, x_1, x_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 $x_{7in} = T_{sus,\,in} \cdot S_T$
- Residence time; can be varied with ξ_{av} dimensionless residence time, where $\xi_{av} = \tau_{mean} \cdot S_t$

Dynamic analysis of the models

Instead of a real unit, the model of the crystalliser – presented above – was stepped in Matlab Simulink environment to collect data for the identification of the model matrix. 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 object was stepped around a stable operating point with reasonable step sizes as tested before.

With the collected data the automated method was use for the model identification in Profit® Design Studio of Honeywell. [10]

The identification result is shown in *Fig. 2*. 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 magnitudes 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, covered.

Profit Design Studio found good models quickly with an automated identification method. All sub-models' qualities are good, Rank 1 or 2 in the range of 1-5, where 1 is the best (model ranking is a standard feature of the package and uses a variety of measures to give an overall rank or "goodness of fit" [10]

The settling time for the process data and the settling time from the calculated transfer function, Settle T and Tf_{Settle} respectively, are close to each other for all sub-models.

In this case the model matrix is full, all the CVs are in connection to all the MVs. 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 the overshoots and high order models would be too sensitive to model error and it would not work in model based controller. These responses are all real but even a slight error in these models (and they will vary in practice as the model is never perfect) will lead to out of phase control which will lead to oscillation. So the oscillation of the models were removed, the simplified robust model is presented in *Fig. 3*, the model is the darker line, the data is the lighter.

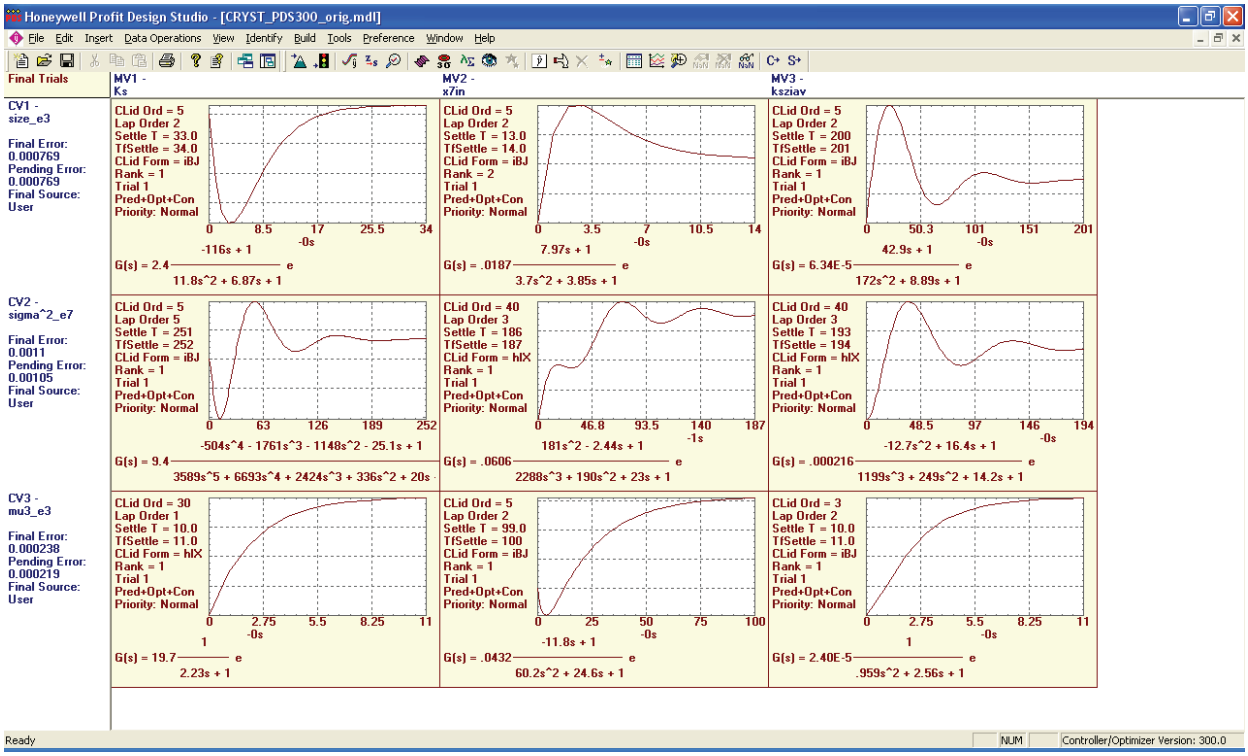

Figure 2: The accurate model matrix

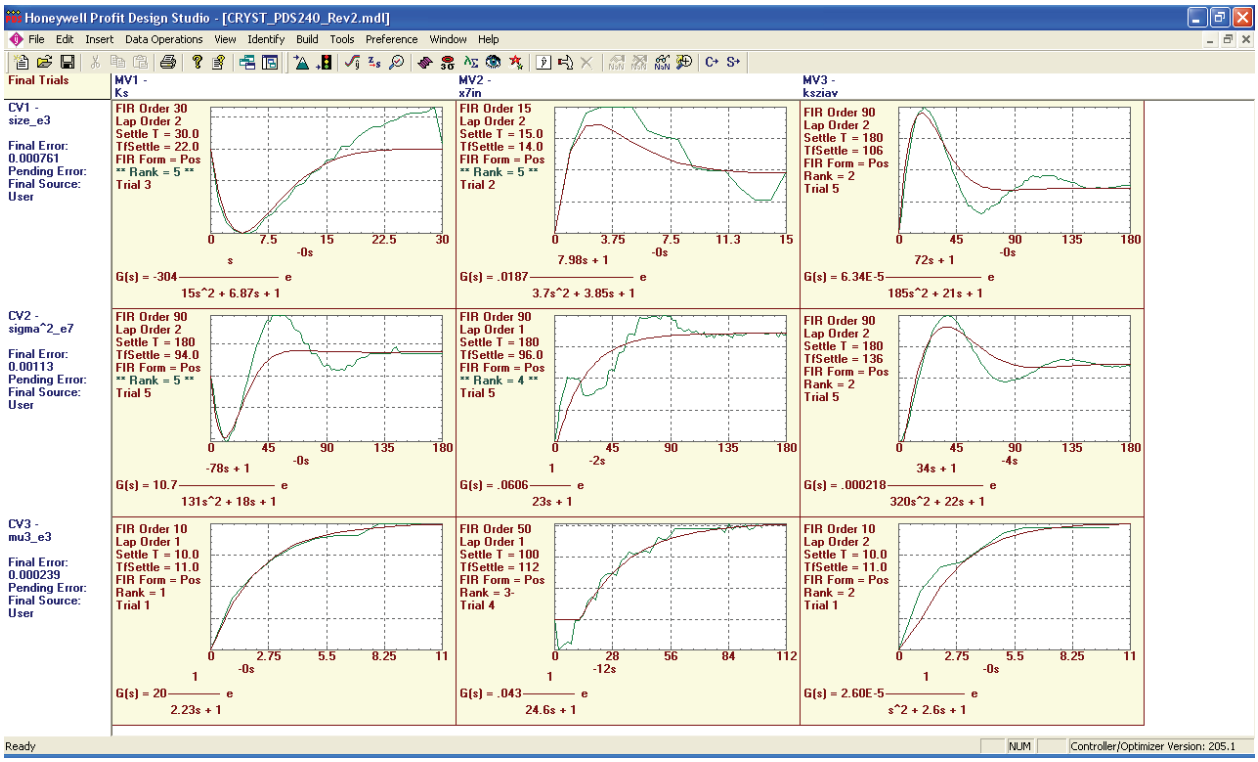

Figure 3: Models used for the control study

The relative gain array was calculated to decide the best pairings.

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 (K):

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

The result of the calculation from the used model matrix (see *Fig. 4*):

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

It is an obvious proof of strong coupling.

Since the best value for pairing is 1 but it shouldn't be negative and 0 [12] the only pairing is the following, showed with bold numbers:

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

So MV1 controls CV3, MV2 controls CV1 and CV2 is controlled by MV3.

Control with PID controllers

First PID controllers were set up and tuned for the vacuum crystalliser.

PID is a single input single output (SISO) controller and as it is showed in that the crystallisers are MIMO object with strong coupling.

The starting points of the PID tunings were calculated with the strategy based on Internal Model Control (IMC). [12]

PID controller in IMC structure:

$$G_c(s) = K_c \left[1 + \frac{1}{s\tau_I} + \tau_D s \right] \tag{9}$$

The filter:

$$F(s) = \frac{1}{\tau_c s + 1} \tag{10}$$

In case of a first order model

$$\left(\frac{K}{\tau s + 1} \right) K_c K = \frac{\tau}{\tau_c}, \ \tau_I = \tau \ \text{ and } \ \tau_D = 0 . \tag{11, 12, 13}$$

The parameters of the PID controllers were finetuned, the MVs were limited, the control structure can be seen in Fig. 4.

The result shows (*Figs 5* and *6*) 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.

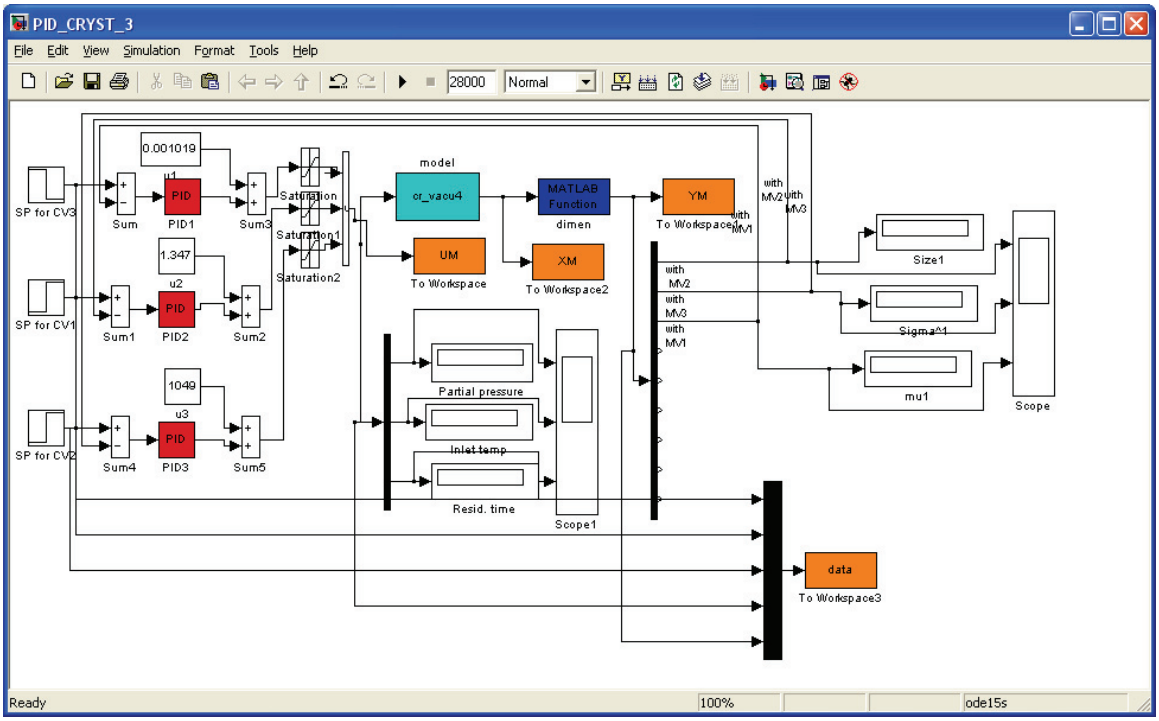

Figure 4: The structure of PID control of the crystalliser model

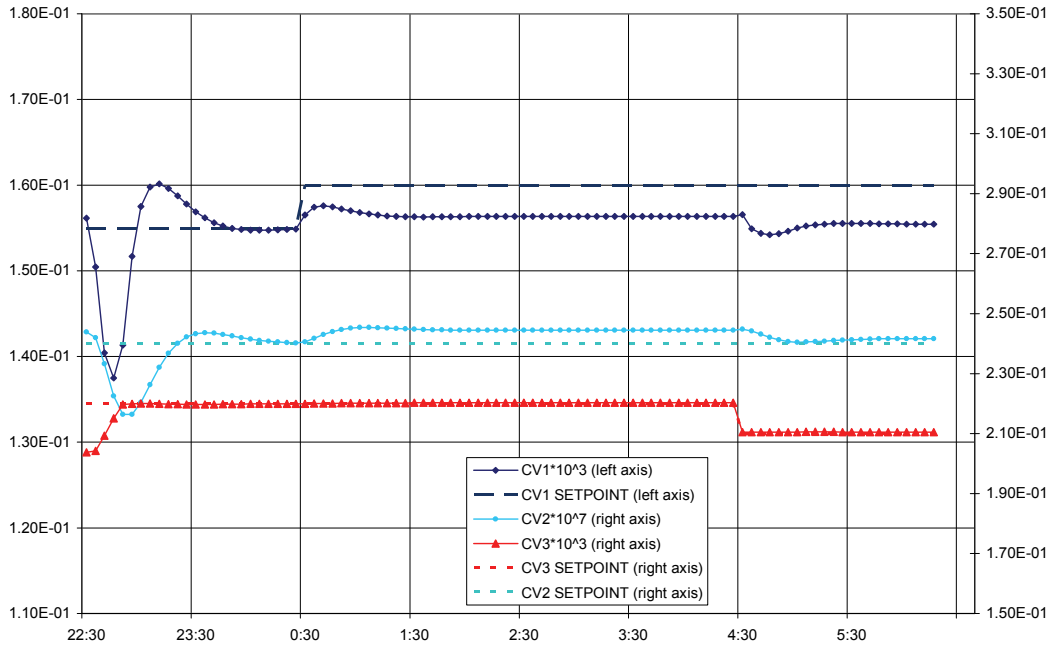

Figure 5: Simulation results with PID controllers, controlled variables
(CV1=crystal size, CV2=crystal size-distribution, CV3=delivery of the crystalliser)

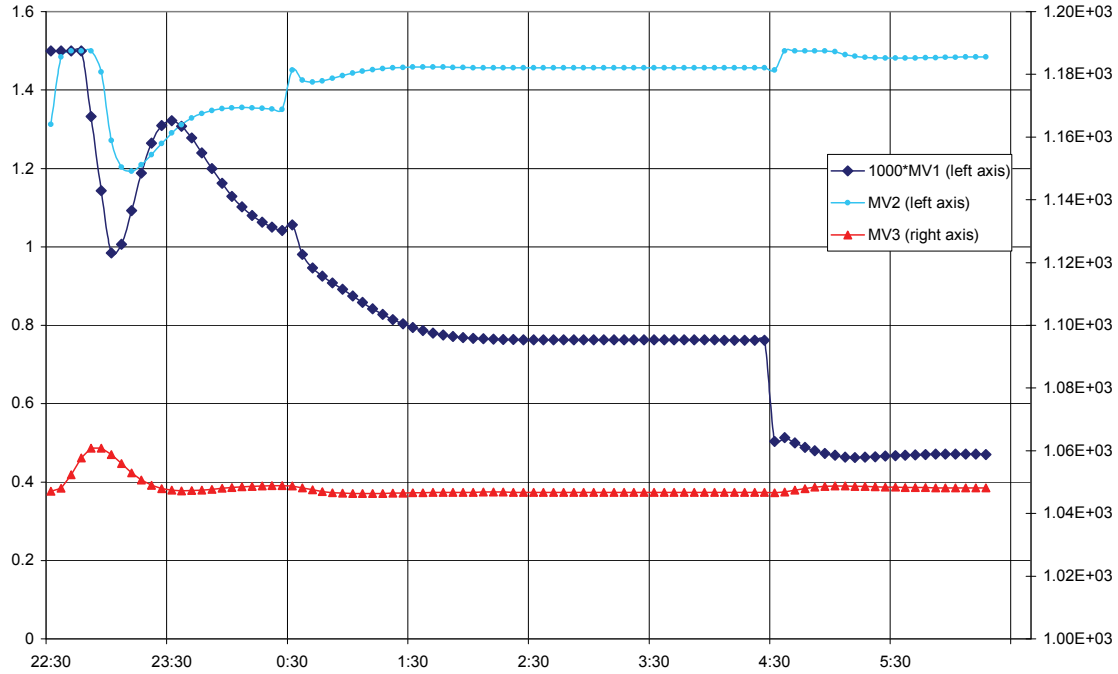

Figure 6: Simulation results with PID controllers, manipulated variables (MV1=pressure, MV2=temperature, MV3=residence time)

It is proved that 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.

To summarise, the above analysed 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 (MPC) presents a good solution. MPC can handle the MIMO object; and it is predictive, so the controller "prevents" over-size crystals.

For non-linearity within a certain range, a robust controller is adequate as it presented below.

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. 7* (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 $\boldsymbol{y} = (\mu_1/\mu_0, \sigma^2, \mu_3)$.

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:

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

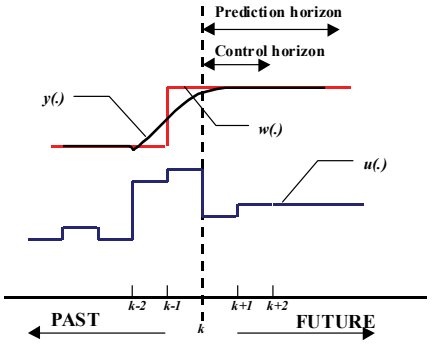

Figure 7: MPC horizons

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 $\hat{y}(k+j|k), j = 1,...H_p$ (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 $u(k+j|k), j = 0,..H_p-1.$, 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 $w(k+j)$, $j = 1,..H_p$ 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. [15]

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) [10]. 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.

Control with MPC

The integration of a process simulator and the MPC of Honeywell was performed with OPC (originally OLE-Object Linking and Embedding for Process Control). 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.

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. 8.*

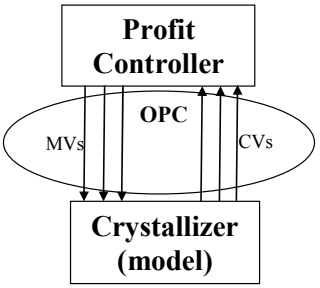

Figure 8: The control shame with Profit Controller

The control horizon (where the manipulated variables changes in the prediction) contains 10 movements of the MVs, in the Honeywell controller, the control horizon for each CV is based on a gain weighted average of the individual models in that row of the matrix.

The prediction horizon (where the prediction is calculated) is the closed loop response interval, this is about 1.5 hours in this case.

Weights, 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 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 cost function is $J= \sigma^2-10\cdot\mu_3$, quadratic coefficients and optimisation of the manipulated variables were not set up.

The optimisation speed factor is 3 (fast), which results in an optimisation horizon approximately 6/3=2 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 minutes in this case.

The simulation results are shown in *Figs 9* and *10.* 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 23:00, from that time the CV3 (delivery) increased significantly, the CV2 (size distribution) deceased a little to the optimal values. CV1 setpoint change is solved after a little overshoot, the changes of MVs (Fig. 10) 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.

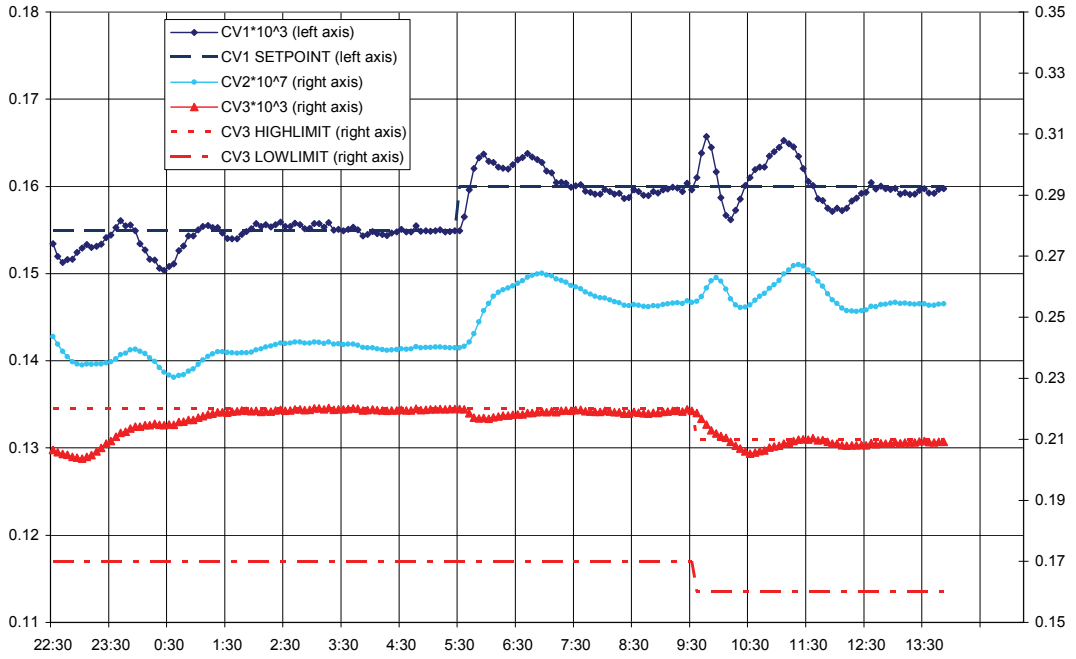

Figure 9: Simulation results for the controller, optimiser, with controlled variables (CV1=crystal size, CV2=crystal size-distribution, CV3=delivery of the crystalliser)

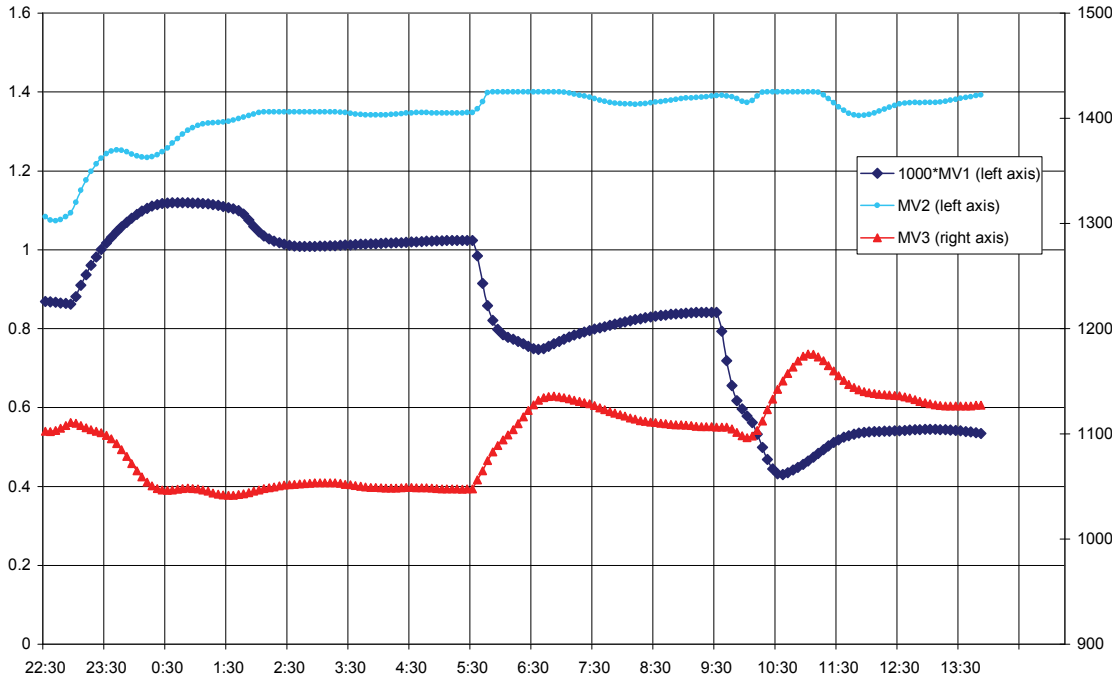

Figure 10: Simulation results for the controller, optimiser, with manipulated variables (MV1=pressure, MV2=temperature, MV3=residence time)

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

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. See *Fig. 11.* 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.

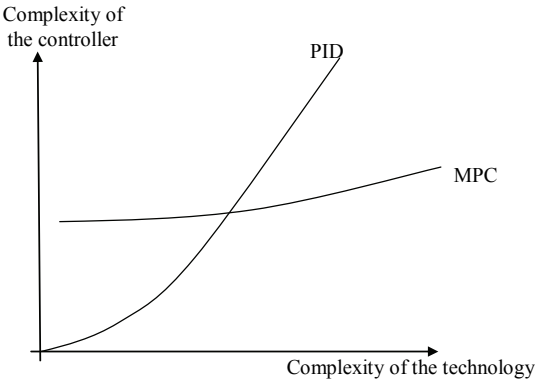

Figure 11: The relationship between the complexity of the technology and the controller

Conclusion

Crystallisers are multivariable objects with coupling among the process variables.

The relative gain array was calculated to try to decouple the input and output variables for the setup of single input single output (SISO) PID controllers. The PIDs were tuned, but the control performance is not satisfying.

Model Predictive Controllers (MPC) can handle such highly interacting multivariable systems efficiently due to their coordinated approach. The feasibility study illustrated that the applied identification tool gave an accurate and robust model, and that the non-linear crystalliser can be controlled and optimised very well with the Honeywell Profit® Suite package. The developed system – engineering model in Matlab is connected to an MPC used in the industry via OPC is proven to be useful in research and development.

ACKNOWLEDGEMENTS

Special thanks to professor Béla Lakatos from the University of Pannonia and colleagues in 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 [9].

Zero order moment:

$$\frac{d\mu_0}{dt} = \frac{F_{sv,in}}{M_{sv}}\left(\mu_{0in} - \mu_0\right) + B + \frac{\mu_0}{M_{sv}}W_v, \quad B = B_p + B_b \tag{A1}$$

First order moment:

$$\frac{d\mu_1}{dt} = \frac{F_{sv,in}}{M_{sv}}\left(\mu_{1,in} - \mu_1\right) + \gamma\left(w_c, w_e\right)\left(\mu_0 + a\mu_1\right) + \frac{\mu_1}{M_{sv}}W_v \tag{A2}$$

Second order model:

$$\frac{d\mu_2}{dt} = \frac{F_{sv,in}}{M_{sv}}\left(\mu_{2,in} - \mu_2\right) + \gamma\left(w_c, w_e\right)\left(\mu_1 + a\mu_2\right) + \frac{\mu_2}{M_{sv}}W_v \tag{A3}$$

Third order model:

$$\frac{d\mu_3}{dt} = \frac{F_{sv,in}}{M_{sv}}\left(\mu_{3,in} - \mu_3\right) + \gamma\left(w_c, w_e\right)\left(\mu_2 + a\mu_3\right) + \frac{\mu_3}{M_{sv}}W_v \tag{A4}$$

Mass balance for solute:

$$\frac{dw_c}{dt} = \frac{F_{sv,in}}{M_{sv}}\left(w_{c,in} - w_c\right) - 3k_V\rho\gamma(w_c - c_s)(\mu_2 + a\mu_3) + \frac{c}{M_{sv}}W_v \tag{A5}$$

Mass balance for the solvent:

$$\frac{dM_{sv}}{dt} = F_{svin} - F_{sv} - W_v \tag{A6}$$

Energy balance equation for the crystal suspension:

$$\frac{dT}{dt} = \frac{F_{svin}}{C_{av}M_{sv}}C_{avin}\left(T_{in} - T\right) - \Delta H_v\frac{W_v}{C_{av}M_{sv}} + 3k_V\rho\gamma(c - c_s)(\mu_2 + a\mu_3)\frac{\Delta H_c}{C_{av}} \tag{A7}$$

where $C_{av} = C_{sv} + Cc + k_V\rho C\mu_3$ and $C_{avin} = C_{sv} + Cc_{in} + k_V\rho C\mu_{3in}$.

Mass balance equation for the vapour phase:

$$\frac{d\rho_v}{dt} = \frac{1}{V_v}\left[\left(1 - \frac{\rho_v}{\rho_{sv}}\right)W_v - \rho_v q_v + \rho_v F_{svin}\left(\frac{1}{\rho_{sv}} + \frac{c_{in}}{\rho} + k_V\mu_{3in}\right) - \rho_v F_{sv}\left(\frac{1}{\rho_{sv}} + \frac{c}{\rho} + k_V\mu_3\right)\right] \tag{A8}$$

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

$$F_v = \rho_v q_v = \rho_v K_s\sqrt{p_v\left(p_v - p_{out}\right)}\,. \tag{A9}$$

Energy balance equation for the vapour phase:

$$\frac{dT_v}{dt} = -\frac{C_v(T_v - T)W_v}{V_v\rho_v\left(C_v + \left(T_v - T\right)\frac{dC_v}{dT_v}\right)}\,. \tag{A10}$$

where:

$$V_v = V - M_{sv}\left(\frac{1}{\rho_{sv}} + \frac{c}{\rho} + k_V\mu_3\right) \tag{A11}$$

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

Temperature dependence of the solubility:

$$c_s\left(T\right) = a_0 + a_1T + a_2T^2 \tag{A12}$$

Evaporation rate of the solvent:

$$W_v = K_{evap}\left(p_v - p_v^*\right) \tag{A13}$$

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

$$\log p_v^* = A_A - \frac{B_A}{T + C_A} \tag{A14}$$

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

$$p_v = \frac{RT_v}{V_v}\,. \tag{A15}$$

NOTATION

a	constant of the crystal growth rate [m^{-1}]
b	exponent of secondary nucleation rate
B_p	primary nucleation rate [no $m^{-3}s^{-1}$]
B_b	secondary nucleation rate [No $m^{-3}s^{-1}$]
c	concentration of solute [kgm^{-3}]
c_s	equilibrium saturation concentration [kgm^{-3}]
D_{ap}	dimensionless parameter for primary nucleation
D_{ab}	dimensionless parameter for secondary nucleation
g	exponent of crystal growth rate
G	crystal growth rate [ms^{-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 [no $m^{-3}s^{-1}$]
k_b	rate coefficient of secondary nucleation [no m^{3b-3} kg^{-b} s^{-1}]
k_V	volume shape factor
L	linear size of crystals [m]
n	population density function [no m^{-4}]
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,...)
x_m	m^{th} order dimensionless moment (m = 0, 1, 2, ...)
y	dimensionless concentration of solute

GREEK LETTERS

ε	viodage of suspension
μ_m	m^{th} order moment of n [m^{m-3}]
ρ_c	density of crystals [kgm^{-3}]
ξ	dimensionless time

SUBSCRIPTS

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

REFERENCES

1. QIN S. J., BADGWELL T. A.: Control Engineering Practice, 11 (2003) 733
2. MYERSON A. S. et al.: Proc. 10th Symposium. Industrial Crystallization. Academia, Praha, 1987
3. JAGER J., et al.: Powder Technology 69 (1992) 11
4. MILLER S. M., RAWLINGS J. B.: AIChE Journal, 40 (1994) 1312
5. ROHANI S. et al.: Computers and Chemical Engineering, 23 (1999) 279.
6. LAKATOS B. G., SAPUNDZHIEV Ts. J.: Bulgarian Chemical Communications, 29 (1997) 28
7. TEMAM R.: Infinite-Dimensional Dynamical Systems in Mechanics and Physics. Springer-Verlag, New York, 1988
8. CHIU T., CHRISTOFIDES P. D.: AIChE Journal, 45 (1999) 1279
9. ULBERT Zs., LAKATOS B. G.: Simulation of CMSMPR vacuum crystallisers. Computers and Chemical Engineering, 23 (1999) S435
10. R300 Profit Suite Documentation, Identifier User's Guide AP09-200, Honeywell International Inc., 2007
11. BRISTOL E. H.: IEEE Trans. on Auto. Control, AC-11, 1966, pp 133-134,
12. COOPER D.: Practical Process Control Using Control Station, Control Station, Inc, Storrs, (2004).CT
13. MEADOWS E. S., RAWLINGS J. B.: Model predictive control, Chapter 5. pp 233-310. Englewoods Cliffs. NJ: Prentice-Hall, 1997
14. JOE QIN S., BADGWELL T. A.: Control Engineering Practice 11 (2003) 733
15. MOLDOVÁNYI N., LAKATOS B. G.: Hungarian Journal of Industrial Chemistry, 33 (2005) 97