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MODEL PREDICTIVE CONTROL OF CONTINUOUS CRYSTALLIZERS

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The problem of model predictive control of continuous isothermal crystallizers, using a detailed moment equation model is analysed. The mean size of the crystalline product and the variance of crystal size are the controlled variables, while the manipulated variables are the input concentration of the solute and the flow-rate. The controllability and observability, as well as the coupling between the inputs and the outputs are analyzed by simulation using the linearised model. The crystallizer has proved to be a nonlinear multi-input multi-output system with strong coupling between the state variables. It is shown that the mean crystal size and the variance of can be controlled nearly separately by the residence time and the inlet solute concentration, respectively. By seeding, the controllability of the crystallizer increases significantly. The linear model predictive controller synthesized using the moment equation model appears to be an efficient controller for continuous crystallizers.

Keywords: Model predictive control; continuous isothermal crystallizer, computer simulation

Introduction

Model predictive control (MPC) refers to a class of computer control algorithms that utilize an explicit process model to predict the future response of the plant. At each control interval an MPC algorithm attempts to optimize future plant behaviour by computing a sequence of future manipulated variable adjustments. The first input in the optimal sequence is then sent into the plant, and the entire calculation is repeated at subsequent control intervals [1]. Originally developed to meet the specialized control needs of power plants and petroleum refineries, MPC technology can now be found in a wide variety of application areas including chemicals (Honeywell has MPC at polypropylene units at TVK, Hungary), food processing (Honeywell is right now working on a dairy product unit at the UK), automotive and aerospace applications. The presented work is an opening to an another new application, the MPC control of continuous crystallizers.

Crystallization is a widely used cleaning, separation and grain producing technique in the chemical industry, particularly at the pharmaceutical works. From the point of view of controlling a crystallizer the main quality criteria are the properties of the produced crystals, first of all the size-distribution and the mean size.

Crystallization is a multi-variable system, with multi input and multi output (MIMO) often with strong coupling. Thus a good, up-to-date control is possible using a model-based MIMO control system. There are only few examples in the literature for this [2-5]. Since one can do nothing to change the size distribution of the crystals in the system once crystals have grown beyond a stable nucleus size. Therefore a predictive type of control would be better than the corrective type. One of the main problems is that for a proper model-based control of the size-distribution, because of the mentioned properties of the population balance equation, high-order control is required, which means serious difficulties. But the crystallizers are dissipative systems [6], so that a crystallizer as a dynamical system possesses finite dimensional global attractors [7] that create an adequate basis for the synthesis and usage of good quality, low-order model-based control systems. At the same time it means that for the synthesis of the model-based control system of crystallizers the moment equation model, generated from population balance equation governing the crystal size distribution can be used. Chui and Cristofides [8] applied this property to design a nonlinear SISO controller.

In this paper a model-based MIMO control system of a continuous isothermal crystallizer is presented. For the synthesis of the control system a multi-variable state-space model is composed. Linear controllability and observability analysis is presented, and the coupling of the inputs and the outputs are analysed. The efficiency of the developed model predictive controller is demonstrated by simulation.

Concept of MPC

In model predictive control, the control action is provided after solving – on-line at each sampling instant – an optimization problem, and the first element in the optimized 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. The major factor of the success of predictive control is its applicability to problems where analytic control law is difficult, or even impossible to obtain.

The methodology of all the controllers belonging to the MPC family is characterized by the following strategy, represented in Fig.1 (y is the output, w is the set-point and u is the input):

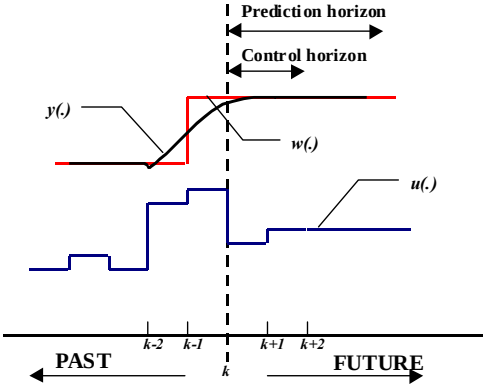

Fig 1. MPC horizons

Prediction horizon (*Hp*) represents the number of samples taken from the future over which MPC computes the predicted process variable profile and minimizes the predicted error. The control signals change only inside the control horizon, *Hc* remaining constant afterwards

$$u(k+j) = u(k+H_c-1), \qquad j = H_c,...,H_p-1 \tag{1}$$

The basic steps:

1. As it is shown, in the MPC future outputs for a determined prediction horizon *Hp* 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 optimizing a cost function in order to keep the process as close as possible to the reference trajectory $w(k+j), j=1,...H_p$. This criterion usually takes the form of a quadratic function of the errors between the predicted output signal and the reference trajectory. The control effort is included in the objective function in most of the cases. An explicit solution can be obtained if the criterion is quadratic, the model is linear and there are no constraints, otherwise an iterative optimization method has to be used.
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 brought up to date. 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.

In order to implement this strategy, the basic structure shown is Fig.2 is used. 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 optimizer taking into account the cost function (where the future tracking error is considered) as well as the constraints.

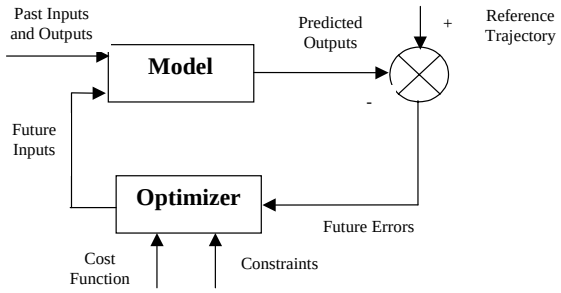

Fig.2: Basic structure of MPC

The process model plays, in consequence, a decisive role in the controller. The chosen model must be capable of capturing the process dynamics so as to precisely predict the future outputs as well as being simple to implement and to understand. As MPC is not a unique technique but a set of different methodologies, there are many types of models used in various formulations. Honeywell uses mostly black-box models at the refineries, getting them by stepping the plant. The new tendency is using chemical engineering, so called "grey-box" models. The presented case study clearly fills this requirement.

The optimizer is another fundamental part of the strategy as it provides the control actions. If the cost function is quadratic, its minimum can be obtained as an explicit function (linear) of past inputs and outputs and the future reference trajectory. In the presence of inequality constraints the solution has to be obtained by more computationally taxing algorithms. The size of optimization problems depends on the number of variables and on the prediction horizon used and usually turn out to be relatively modest optimization problems which do not require sophisticated computer codes to be solved. However the amount of time needed for the constrained and robust cases can be various orders of magnitude higher than that needed for the unconstrained case and

the bandwidth of the process to which constrained MPC can be applied is considerably reduced.

For a continuous-time model (the cost function is discrete), the MPC problem can be represented as

$$\min_{U(k)} J = \Psi\left[Y(k), U(k)\right], \tag{2}$$

$$\hat{x}(t^*) = f\left[x(t^*), u(t^*)\right], \qquad t \le t^* \le t + H_p \Delta t \tag{3}$$

$$u(t^*) = u\left[t + (H_c - 1)\Delta t\right], t + (H_c - 1)\Delta t \le t^* \le t + H_p \Delta t$$

$$0 = \Phi\left[X(k), Y(k), U(k)\right], \tag{5}$$

$$0 \ge DU(k) \tag{6}$$

$$0 \ge DY(k) \tag{7}$$

where

$$U(k) \equiv \begin{bmatrix} u(k|k) \\ u(k+1|k) \\ \vdots \\ u(k+H_c-1|k) \end{bmatrix}, \qquad Y(k) \equiv \begin{bmatrix} y(k|k) \\ y(k+1|k) \\ \vdots \\ y(k+H_p|k) \end{bmatrix},$$

$$X(k) \equiv \begin{bmatrix} x(k|k) \\ x(k+1|k) \\ \vdots \\ x(k+H_p|k) \end{bmatrix}.$$

Here, $u(k|k)$ is the input $u(k)$ calculated from information available at time *k*, $y(k|k)$ is the output $y(k)$ calculated from information available at time *k*, *Hc* is the control horizon and *Hp* is the prediction horizon, while *x* denotes the state variable. Constraint (3) corresponds to satisfaction of the continuous-time model equations over the prediction horizon, while (4) enforces the requirement that all inputs beyond the control horizon are held constant. Algebraic equation (5) represents constraints for the model, and for the sake of completeness Eqs (6) and (7) correspond to the constraints on the input and output variables, respectively.

The process model is assumed to have the following discrete-time representation,

$$x(k+1) = F\left[x(k), u(k),\right] \tag{8}$$

$$y(k) = h\left[x(k)\right], \tag{9}$$

where *x* is the *n*-dimensional vector of state variables, *u* is the *m*-dimensional vector of manipulated input variables, and *y* is the *p*-dimensional vector of controlled output variables. Such a model can be obtained by discretizing a continuous-time, state-space model or by deriving a state-space realization of a discrete-time, input-output model. It is important to note that time delays can be handled by augmenting the state vector such that the resulting state-space model has no delays.

The optimization problem for the prototypical MPC formulation is [9]:

$$\min_{u(k|k),u(k+1|k),\ldots u(k+H_c-1|k)} J = \phi\left[y(k+H_p|k)\right] + \sum_{j=0}^{H_p-1} L\left[y(k+j|k), u(k+j|k), \Delta u(k+j|k)\right], \tag{10}$$

where $\Delta u(k+j|k) = u(k+j|k) - u(k+j-1|k)$, ϕ and L are (possibly) (non)linear functions of their arguments. The optimization problem is solved to the constraints discussed below. The functions ϕ and L can be chosen to satisfy a wide variety of objectives, including minimization of overall process cost. However, economic optimization may be performed by a higher-level system which determines appropriate setpoints for the MPC controller. In this case it is meaningful to consider quadratic functions of the following form:

$$L = \left[\mathrm{y(k+j|k)} - y_s(k)\right]^T Q\left[\mathrm{y(k+j|k)} - y_s(k)\right] + \left[\mathrm{u(k+j|k)} - u_s(k)\right]^T R\left[\mathrm{u(k+j|k)} - u_s(k)\right] + \Delta u^T(\mathrm{k+j|k}) S \Delta u(\mathrm{k+j|k}), \tag{11}$$

$$\phi = \left[y(\mathrm{k+H_p|k}) - y_s(k)\right]^T Q\left[y(\mathrm{k+H_p|k}) - y_s(k)\right] \tag{12}$$

where $u_s(k)$ and $y_s(k)$ are steady-state targets for *u* and *y*, respectively, and *Q, R, S* are positive definite weighting matrices. The principal controller tuning parameters are *Hc, Hp, Q, R, S* and the sampling period Δt.

The prediction outputs are obtained from the model (8-9). Successive iterations of the model equations yield

$$\begin{aligned} y(k+1|k) &= h\left[x(k+1|k)\right] = h\left[F\left[x(k|k), u(k|k)\right]\right], \\ &\equiv G_1\left[x(k), u(k|k)\right], \\ y(k+2|k) &= G_1\left[x(k+1|k), u(k+1|k)\right], \\ &\equiv G_1\left[F\left[x(k|k), u(k|k)\right], u(k+1|k)\right], \\ &\equiv G_2\left[x(k), u(k|k), u(k+1|k)\right], \\ &\vdots \\ y(k+j|k) &= G_j\left[x(k), u(k|k), u(k+1|k), \ldots u(k+j-1|k)\right], \end{aligned} \tag{13}$$

where $x(k|k) = x(k)$ is a vector of current state variables. If the control horizon (*Hc*) is less than the prediction horizon (*Hp*), the output predictions are generated by setting inputs beyond the control horizon equal to the last computed value:

$$u(k+j|k) = u(k+H_c-1|k), \qquad H_c \le j \le H_p.$$

Note that the prediction $y(k+j|k)$ depends on the current stable variables, as well as on the calculated input sequence. Therefore, MPC requires measurements or estimates of the state variables.

Solution of the MPC problems yields the input sequence $\left\{u(k|k), u(k+1|k), \ldots, u(k+H_c-1|k)\right\}$ Only the first input vector in the sequence is actually implemented: $u(k) = u(k|k)$. Then the prediction horizon is moved forward one time step, and the problem is resolved using new process measurements. This receding horizon formulation yields improved closed-loop performance in the presence of unmeasured disturbances and modelling errors.

Case Study: Continuous crystallizer

Moment equation model

The mathematical model of a continuous MSMPR crystallizer consists of the population balance equation for crystals, of the balance equations for sol-vent and crystallizing substance, and of the equations describing the variation of the equilibrium saturation concentration. In the present analysis, the crystallizer is assumed to be isothermal, thus the equilibrium saturation concentration c^* is constant during the course of the process.

It is assumed that the following conditions are satisfied:

(1) the volumetric feed and withdrawal rates of the crystallizer 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 $L_n \cong 0$ so that we 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

$$G = k_g (c - c^*)^g (1 + aL); \tag{14}$$

(7) the primary nucleation rate B_p is described by the Volmer model

$$B_p = k_p \varepsilon \exp\left(-\frac{k_e}{\ln^2\left(\frac{c}{c^*}\right)} \right) \tag{15}$$

the secondary nucleation rate Bs is described by the power law relation

$$B_b = k_b (c - c^*)^b \mu_3^j \tag{16}$$

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

$$\mu_m = \int_0^\infty L^m n(L,t) dL, m = 0,1,2,3... \tag{17}$$

With these assumptions the population balance equation governing the crystal size dynamics becomes:

$$V\left(\frac{\partial n(L,t)}{\partial t} + \frac{\partial \left[G(c,L,c^*) n(L,t) \right]}{\partial L} \right) = q\left[n_{in}(L,t) - n(L,t) \right]$$
$$t > 0,\ L > 0 \tag{18}$$

subject to the following initial and boundary conditions:

$$n(L,0) = n_0(L), \quad L \geq 0 \tag{19}$$

$$\lim_{L \to 0} G(c,L,c^*) n(L,t) = B_v(c,c^*), \quad v = p,b \quad t \geq 0 \tag{20}$$

$$\lim_{L \to \infty} n(L,t) = 0, \quad t \geq 0 \tag{21}$$

Here, $n(L,t)\mathrm{d}L$ expresses the number of crystals having sizes in the range L to $L+\mathrm{d}L$ at time t in a unit volume of suspension.

The mass balance of the crystallizing substance has the form

$$V \frac{d\left[\varepsilon c + (1-\varepsilon)\rho_c \right]}{dt} = q c_{in} - q\left[\varepsilon c + (1-\varepsilon)\rho_c \right] \tag{22}$$

with the initial condition

$$c(0) = c_0 \tag{23}$$

where the voidage of suspension ε is related to n and L by

$$\varepsilon = 1 - k_V \mu_3 = 1 - k_V \int_0^\infty L^3 n(L,t) dL \tag{24}$$

Finally, the mass balance of the solvent is written in the form

$$V \frac{d\left(\varepsilon c_{sv} \right)}{dt} = q c_{svin} - q \varepsilon c_{sv} \tag{25}$$

with the initial condition

$$c_{sv}(0) = c_{sv0}\,. \tag{26}$$

Therefore, the state at time $t \geq 0$ of the continuous isothermal MSMPR crystallizer is given by the triple $[c(t), c_{sv}(t), n(t)]$, and its dynamics is described by the distributed parameter model formed by the mixed set of partial and ordinary differential eqs (18), (22) and (25), subject to the initial and boundary conditions (19-21) (23) and (26). The evolution in time of this system occurs in the state space $\boldsymbol{R}^2 \times \boldsymbol{N}$ that is the Descartes product of the vector space $\boldsymbol{R}^2$ of concentrations and of the function space $\boldsymbol{N}$ of the population density functions. Consideration of dynamical problems of crystallizers in this product space, however, seems to be quite complex and not constructive. In the present study, we concentrate on a reduced case, considering the problem in a finite dimensional state space model based on the moments of the population density function instead of the distributed parameter system (18)-(21).

Since the overall crystal growth rate (14) is a linear function of size L, the population balance Eq. (18) can be converted into an infinite set of recursive ordinary differential equations for the moments of population density function:

$$V \frac{d\mu_0}{dt} = q\left(\mu_{0in} - \mu_0 \right) + V B_v, \quad v = p,b \tag{27}$$

$$V \frac{d\mu_m}{dt} = q\left(\mu_{\min} - \mu_m \right) + V m k_g (c - c^*)^g (\mu_{m-1} + a\mu_m)$$
$$m=1,2,3 \tag{28}$$

which can be closed by Eq.(22), describing the mass balance of the crystallizing substance, at the equation for the third order moment. Then Eq.(22) takes the form

$$V \frac{dc}{dt} = \frac{q}{\varepsilon}(c_{in} - c) - \frac{1}{\varepsilon} 3 k_V k_g V (\rho_c - c)(c - c^*)^g (\mu_2 + a\mu_3) \tag{29}$$

while Eq.(12) can be rewritten as

$$V \frac{dc_{sv}}{dt} = \frac{q}{\varepsilon}(c_{svin} - c_{sv}) - \frac{1}{\varepsilon} 3 k_V k_g V c_{sv} (c - c^*)^g (\mu_2 + a\mu_3) \tag{30}$$

where c_{sv} stands for the concentration of solvent. Here, because of the selective withdrawal, the voidage in the crystallizer and that in the outlet stream are not equal.

Therefore, the first four moment equations from the system (27-28) with Eqs (29-30) provide a closed moment equations model of the crystallizer.

Dimensionless equations. Scaling

We introduce the following set of dimensionless variables

$$\xi = s_t t,\ x_m = s_m \mu_m,\ m = 0,1,2,3,\ y = s_c (c - c^*),$$
$$y_{in} = s_c (c_{in} - c^*),\ y_{sv} = s_c c_{sv},\ y_{svin} = s_c c_{svin}$$

into Eqs (27)-(30), where s_t, s_c and s_m, m=0,1,2,3, are scale factors defined as

$$s_c := \frac{1}{\max\{c_{in}\} - c^*},\ s_0 := 6k_V k_g^3 s_t^{-3} \left(\max\{c_{in}\} - c^*\right)^{3g}$$
$$s_1 := 6k_V k_g^2 s_t^{-2} \left(\max\{c_{in}\} - c^*\right)^{2g}$$
$$s_2 := 3k_V k_g s_t^{-1} \left(\max\{c_{in}\} - c^*\right)^{g},\quad s_3 := k_V$$

and $\max\{c_{in}\}$ denotes the maximal value of inlet concentration, as well as the set of dimensionless parameters

$$\tau := s_t \bar{t} = s_t \frac{V}{q},\ \alpha := (\rho - c^*)\left(\max\{c_{in}\} - c^*\right)^{-1}$$
$$\beta := k_g a s_t^{-1} \left(\max\{c_{in}\} - c^*\right)^{g}$$
$$D_{ap} := 6k_p k_V k_g^3 s_t^{-4} \left(\max\{c_{in}\} - c^*\right)^{3g}$$
$$D_{ab} := 6k_b k_V^{1-j} k_g^3 s_t^{-4} \left(\max\{c_{in}\} - c^*\right)^{3g+b}$$
$$\gamma := s_c c^* = \frac{c^*}{\max\{c_{in}\} - c^*}$$

Then the dimensionless governing equations take the form:

$$\frac{dx_0}{d\xi} = \frac{x_{0in} - x_0}{\tau} + \Theta_\nu,\quad \nu = p, b \tag{31}$$

$$\frac{dx_m}{d\xi} = \frac{x_{\min} - x_m}{\tau} + y^g (x_{m-1} + m\beta x_m),\ m = 1,2,3 \tag{32}$$

$$\frac{dy}{d\xi} = \frac{y_{in} - y}{\tau(1 - x_3)} - \frac{(\alpha - y) y^g (x_2 + 3\beta x_3)}{1 - x_3} \tag{33}$$

$$\frac{dy_{sv}}{d\xi} = \frac{y_{svin} - y_{sv}}{\tau(1 - x_3)} + \frac{y_{sv} y^g (x_2 + 3\beta x_3)}{1 - x_3} \tag{34}$$

subject to the initial conditions

$$x_m(0) = x_{m0},\ m = 0,1,2,3,\quad y(0) = y_0,\quad y_{sv}(0) = y_{sv0}$$

where

$$\Theta_p = D_{ap}(1 - x_3) \exp\left(- \frac{k_e}{\ln^2\left(\frac{y + \gamma}{\gamma}\right)} \right) \tag{36}$$

and

$$\Theta_b = D_{ab} y^b x_3^j . \tag{37}$$

It follows from physical reasoning that the physically admissible solutions to Eqs (31-34) should satisfy the constraints

$$0 \le y \le y_{in},\quad 0 \le x_0 \le x_{0m},\quad 0 \le x_1 \le A_1 x_{0m}^{\frac{2}{3}},$$
$$0 \le x_2 \le A_2 x_{0m}^{\frac{1}{3}},\quad 0 \le x_3 < x_{3\max} = 1 - \varepsilon_{\min} < 1 \tag{38}$$

where x_{0m} denotes the maximal value of the zero order moment, while

$$\varepsilon_{\min} = \frac{V_{sv}}{V\left(1 - \frac{c^*}{\rho}\right)} \tag{39}$$

where V_{sv} is the volume of solvent in the crystallizer.

The parameters, which in the case of primary and secondary nucleation form the vectors of real numbers $p_p=(\tau,\alpha,g,\beta,Dap,ke,\gamma)$ and $p_b=(\tau,\alpha,g,\beta,Dab,b,j)$, respectively, are also bounded:

$$\tau \ge 0,\ \alpha \ge 0,\ g \ge 0,\ \beta \ge \beta_{\min},\ D_{ap} \ge 0,\ D_{ab} \ge 0$$
$$k_e \ge 0,\ b \ge 0,\ j \ge 0,\ \gamma \ge 0 \tag{40}$$

As a consequence, the state of crystallizer (31)-(34) is represented by the vector of variables (x_0,x_1,x_2,x_3,y, y_{sv}), and its time evolution occurs in the feasible region of solutions (38) of the six-dimensional state space $\boldsymbol{R}^6$.

The behaviour of crystallizer in the neighbourhood of a stationary state may be deduced by examining the eigenvalues of the Jacobian matrix of Eqs (36-38) at this state which becomes

$$\begin{bmatrix}
-\frac{1}{\tau} & 0 & 0 & j_{14vS} & j_{15vS} & 0 \\
y_S^g & \beta y_S^g - \frac{1}{\tau} & 0 & 0 & g\frac{(x_{1S} - x_{1in})}{\tau y_S} & 0 \\
0 & y_S^g & 2\beta y_S^g - \frac{1}{\tau} & 0 & g\frac{(x_{2S} - x_{2in})}{\tau y_S} & 0 \\
0 & 0 & y_S^g & 3\beta y_S^g - \frac{1}{\tau} & g\frac{(x_{3S} - x_{3in})}{\tau y_S} & 0 \\
0 & 0 & -\frac{(\alpha - y_S) y_S^g}{1 - x_{3S}} & -\frac{3\beta(\alpha - y_S) y_S^g}{1 - x_{3S}} & j_{55S} & 0 \\
0 & 0 & -\frac{y_{svS} y_S^g}{1 - x_{3S}} & -\frac{3\beta y_{svS} y_S^g}{1 - x_{3S}} & -\frac{g(y_{svin} - y_{svS})}{y_S(1 - x_{3S})} & -\frac{1 + x_{3S}}{\tau(1 - x_{3S})}
\end{bmatrix} \tag{41}$$

where in the case of primary nucleation

$$j_{14pS} = \frac{x_{0in} - x_{0S}}{\tau(1 - x_{3S})} \quad \text{and} \quad j_{15pS} = \frac{2k_e(x_{0S} - x_{0in})}{\tau(y_S + \gamma)\ln^3\left(\frac{y_S + \gamma}{\gamma}\right)} \tag{42}$$

$$j_{55S} = \frac{1}{1 - x_{3S}} \left[-\frac{1}{\tau} + \frac{(y_{in} - y_S)[y_S - g(\alpha - y_S)]}{\tau y_S (\alpha - y_S)} \right]$$

while for secondary nucleation

$$j_{14sS} = j\frac{x_{0S}}{x_{3S}} \quad \text{and} \quad j_{15sS} = s\frac{x_{0S}}{y_S} \tag{43}$$

In order to formulate the state-space model, we define

$$\boldsymbol{u} = (x_{0in}, x_{1in}, x_{2in}, x_{3in}, y_{in}, w) = (u_1, u_2, u_3, u_4, u_5, u_6) \tag{44}$$

where

$$w = s_q q = \frac{V}{\tau} s_t s_q = \frac{V s_V}{\tau} = \frac{\Omega}{\tau} . \tag{45}$$

Now:

$$\frac{dx_0}{d\xi} = w\frac{x_{0in} - x_0}{\Omega} + \Theta_\nu, \quad \nu = p,b \tag{46}$$

$$\frac{dx_m}{d\xi} = w\frac{x_{\min} - x_m}{\Omega} + y^g(x_{m-1} + m\beta x_m)$$

m=1,2,3 (47)

$$\frac{dy}{d\xi} = w\frac{y_{in} - y}{\Omega(1-x_3)} - \frac{(\alpha - y)y^g(x_2 + 3\beta x_3)}{1-x_3} \tag{48}$$

$$\frac{dy_{sv}}{d\xi} = w\frac{y_{svin} - y_{sv}}{\Omega(1-x_3)} - \frac{y_{sv}y^g(x_2 + 3\beta x_3)}{1-x_3} \tag{49}$$

subject to the initial conditions

$$x_m(0) = x_{m0},\ m = 0,1,2,3, \quad y(0) = y_0, \quad y_{sv}(0) = y_{sv0} \tag{50}$$

i.e.

$$\frac{dx_0}{d\xi} = u_6\frac{u_1 - x_0}{\Omega} + \Theta_\nu, \quad \nu = p,b \tag{51}$$

$$\frac{dx_m}{d\xi} = u_6\frac{u_m - x_m}{\Omega} + y^g(x_{m-1} + m\beta x_m),\ m=1,2,3 \tag{52}$$

$$\frac{dy}{d\xi} = u_6\frac{u_5 - y}{\Omega(1-x_3)} - \frac{(\alpha - y)y^g(x_2 + 3\beta x_3)}{1-x_3} \tag{53}$$

$$\frac{dy_{sv}}{d\xi} = u_6\frac{y_{svin}(u_5) - y_{sv}}{\Omega(1-x_3)} - \frac{y_{sv}y^g(x_2 + 3\beta x_3)}{1-x_3} \tag{54}$$

where

$$y_{svin} = \rho_{sv}\left(s_c - \frac{y_{in}}{\rho}\right) = \rho_{sv}\left(s_c - \frac{u_5}{\rho}\right) \tag{55}$$

To summarize as a control engineering problem: vector of state-variables is $\boldsymbol{x}=(x_0,x_1,x_2,x_3,,y,y_{sv})$, its changes represented by a nonlinear state space model (51)-(55); the input vector of is $\boldsymbol{u}=(x_{0in},x_{1in},x_{2in},x_{3in},y_{in},w)$ and the output is defined as $\boldsymbol{y}=\boldsymbol{x}$.

Analysis of the model

Stability and bifurcation

In linear dynamics, one seeks the fundamental solutions from which one can build all other solutions. In nonlinear dynamics, the main questions are: What is the qualitative behaviour of the system? Which and how many non-wandering sets (i.e. a fixed point, a limit cycle, a quasi-periodic or chaotic orbit) occur? Which of them are stable? How does the number of non-wandering sets change while changing a parameter of the system (called control parameter)? The appearance and disappearance of a non-wandering set is called a bifurcation. Change of stability and bifurcation always coincide.

The number of attractors in a nonlinear dynamical system can change when a system parameter is changed. This change is called bifurcation. It is accompanied by a change of the stability of an attractor. In a bifurcation point, at least one eigenvalue (λ) of the Jacobian matrix gets a zero real part. There are three generic types of so-called co-dimension-one bifurcations (the term co-dimension counts the number of control parameters for which fine tuning is necessary to get such a bifurcation).

Back to the crystallizer, changing the value of k_e, the parameter of primary nucleation rate and observing the supersaturation, Hopf bifurcation occurs as it shown in Fig.3.

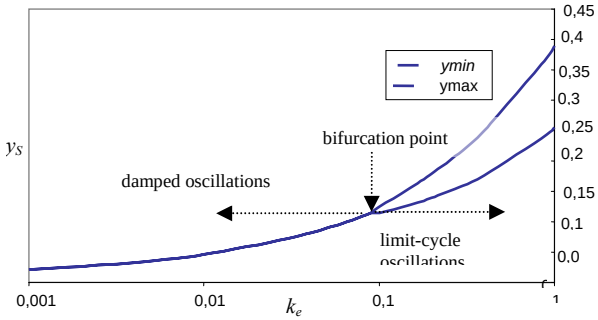

Fig. 3: Bifurcation diagram k_e-y_S of the crystallizer

For further studies of controlling the crystallizer an operating point has been chosen from the region of stable steady states exhibiting only damped oscillations, that is at k_e=0.01.

Controllability and observability

There are two basic problems we need to consider. The first one is the coupling between the input and the state: Can any state be controlled by the input? This is a controllability problem. Another is the relationship between the state and the output: Can all the information about the state be observed from the output? This is an observability problem.

For the controllability and observability test a linearized model (at the operating point) of the nonlinear system was used.

$$\begin{aligned} \dot{\boldsymbol{x}} &= \boldsymbol{A}\boldsymbol{x} + \boldsymbol{B}\boldsymbol{u} \\ \boldsymbol{y} &= \boldsymbol{c}^T\boldsymbol{x} \end{aligned} \tag{56}$$

where the state transition matrix ($\boldsymbol{A}$) is the Jacobi matrix of the system, the input matrix ($\boldsymbol{B}$) can also be derived from the model and the output matrix ($\boldsymbol{c}^T$) is a diagonal matrix.

For a MIMO system the necessary and sufficient conditions for the system to have completely controllability is

$$Rank\left[\mathbf{B}\middle|\mathbf{AB}\middle|\mathbf{A^2B}\middle|\cdots\middle|\mathbf{A^{n-1}B}\right] = n \tag{57}$$

For the general system the necessary and sufficient condition of a linear system for complete observability is

$$Rank\left[\mathbf{c}\middle|\mathbf{A}^T\mathbf{c}\middle|(\mathbf{A}^T)^2\mathbf{c}\middle|\cdots\middle|(\mathbf{A}^T)^{n-1}\mathbf{c}\right]^T = n \tag{58}$$

The results of the calculation is that the linearized system is completely controllable and observable at a certain operating point.

Relative –gain array

The relative-gain array provides exactly a methodology, whereby we select pairs of input and output variables in order to minimize the amount of iteration among the resulting loops. It was first proposed by Bristol and today is a very popular tool for the selection of control loops.

In our crystallization system the control variables can be the mean size of crystals, the variance of the crystal size (σ^2) and the productivity, i.e. the total volume of the crystals:

$$\upsilon_1 = \frac{x_1}{x_0}, \quad \upsilon_2 = \frac{x_2}{x_0} - \left(\frac{x_1}{x_0}\right)^2, \quad \upsilon_3 = x_3 \tag{59}$$

The manipulated variables are the input concentration of the solute and the flow-rate:

$$\vartheta_1 = u_5 = y_{in}, \quad \vartheta_2 = u_6 = w. \tag{60}$$

For the crystallizer we have two outputs and two inputs, there are three possible pairs of control variables, so three different relative-gain arrays can be formed and computed (The value 0 and 1 are rounded.):

$$\begin{bmatrix} \Delta\upsilon_1 \\ \Delta\upsilon_2 \end{bmatrix} = \begin{bmatrix} 128.21 & -127.21 \\ -127.21 & 128.21 \end{bmatrix} \begin{bmatrix} \Delta\vartheta_1 \\ \Delta\vartheta_2 \end{bmatrix}$$

$$\begin{bmatrix} \Delta\upsilon_1 \\ \Delta\upsilon_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \Delta\vartheta_1 \\ \Delta\vartheta_2 \end{bmatrix}, \quad \begin{bmatrix} \Delta\upsilon_2 \\ \Delta\upsilon_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \Delta\vartheta_1 \\ \Delta\vartheta_2 \end{bmatrix}$$

The results show that controlling the mean size and the variance together would be very difficult. However, by putting crystal grains to the input (seeding), the control of the variance also becomes possible. The new different relative-gain array:

$$\begin{bmatrix} \Delta\upsilon_1 \\ \Delta\upsilon_2 \end{bmatrix} = \begin{bmatrix} 1.24 & -0.24 \\ -0.24 & 1.24 \end{bmatrix} \begin{bmatrix} \Delta\vartheta_1 \\ \Delta\vartheta_2 \end{bmatrix}$$

In this case, the mean-size and the variance can be nearly separately controlled. For the further experiments these two outputs will be selected. The system is very sensible to the quality and the quantity of the seeding. It is assumed to be fixed to a suitable operating point.

Results of simulations

The cost function is chosen to satisfy a wide variety of objectives, including minimization of overall process costs. However, economic optimization may be performed by a higher-level system which determinates the appropriate setpoints for the controller. In this case cost function is formulated reflecting the reference tracking error and the control action. The general expression of such an objective function is

$$J(H_{p1}, H_{p2}, H_c, \boldsymbol{R}, \boldsymbol{Q}) = \sum_{j=H_{p1}}^{H_{p2}} (\boldsymbol{w}(k+j) - \hat{\boldsymbol{y}}(k+j))^T \boldsymbol{Q} (\boldsymbol{w}(k+j) - \hat{\boldsymbol{y}}(k+j)) + \sum_{j=1}^{H_c} \boldsymbol{\Delta u}(k+j-1)^T \boldsymbol{R} \boldsymbol{\Delta u}(k+j-1) \tag{61}$$

where $\hat{\boldsymbol{y}}(k+j)$ denotes the predicted process outputs, H_{p1} and H_{p2} are the minimum and the maximum prediction horizons, H_c is the control horizon, Q and R are positive definite weighting matrices.

An optimization algorithm will be applied to compute a sequence of future control signals that minimizes the cost function. For unconstrained control based on linear process model(s) and quadratic cost function the control sequence can be analytically calculated. After tuning the $H_c = 3$, the $H_{p1} = 1$ and $H_{p2} = 5$.

By seeding, the controllability of the crystallizer increase, the overshoots and the oscillation are smaller. The results of the controlling study have shown that the linear MPC is an adaptable and feasible controller as it illustrated by Fig.4. Here, the first two rows are the outputs (solid lines) with the corresponding setpoints (dashed lines), while the third and fourth rows present the time variations of the inputs of the crystallizer. Note that since the volume of the crystal suspension was kept constant the mean residence time was varied by changing the volumetric feed.

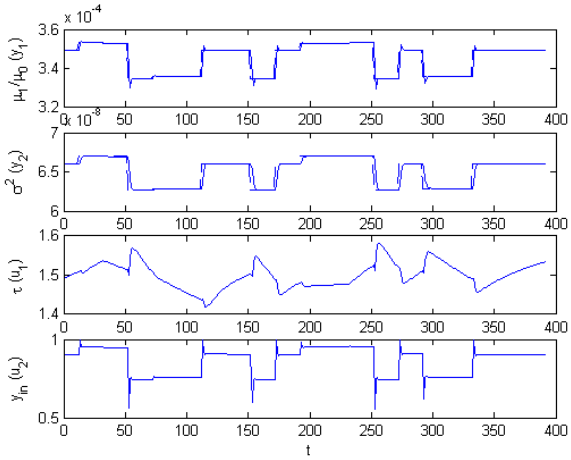

Fig.4. Performance of the MPC of the continuous isothermal MSMPR crystallizer

Next steps

The presented model is going to be developed in UniSim, the simulation software of Honeywell, to make possible to connect it to the Profit Controller. the MPC of Honeywell. The final step is to control a real continuous crystallizer at a plant.

Conclusions

The moment equation model of a continuous isothermal MSMPR crystallizer was presented and the model was analyzed. Better control of the variance of the crystal size was possible by introducing some seeding into the crystallizer. By seeding, the controllability of the crystallizer increase, the overshoots and the oscillation are smaller. The results of the controlling study have shown that the linear MPC is an adaptable and feasible controller for continuous crystallizers.

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