

AN INDUSTRIAL MODEL PREDICTIVE CONTROL ARCHITECTURE FOR BATCH CRYSTALLISATION

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This paper describes an industrial Model Predictive Control (MPC) architecture for batch crystallisation processes. The architecture consists of an industrial model predictive controller (INCA[®], IPCOS), an observer (Extended Kalman Filter / Luenberger type), a non-linear moment model of a batch crystalliser and an OPC communication interface. Presented is how the architecture can be used to achieve maximum throughput of a batch crystallisation process, while satisfying requirements on product quality. Proper control of the crystal growth rate in the batch crystallisation process is the key to fulfilment of this objective. Simulation and experimental results are presented of the framework applied to a seeded fed-batch evaporative 75-l draft-tube crystalliser of ammonium sulphate.

1. Introduction

The fierce competition in today's economy has forced companies to produce high added-value products, while their production processes should show a high production rate of within-specification materials and have a reproducible character (low variability).

Batch crystallisation is an unit operation in process industry often employed for production of high purity, high added-value materials with tight specifications on the final product quality. The quality of crystalline products can be characterised by several different aspects, e.g. purity of the crystals, morphology (crystal habit) and Crystal Size Distribution (CSD). A quantitative description of the relation between product quality and process conditions during crystallisation is difficult to find. However, the crystal growth rate is considered as the most critical process parameter having a close relation with a majority of the quality aspects. High crystal growth rates will lead to more impurity uptake in the crystal, more liquid inclusions, agglomeration and nucleation. All these phenomena have a negative effect on the crystal quality aspects. Crystallisation processes are known to be operated within the metastable region, which translates to limiting the supersaturation level in the crystalliser and indirectly the crystal growth rate. Given these considerations, a low crystal growth rate is favourable. On the other hand, achieving a high throughput of the crystallisation process requires a maximal crystal growth rate. This namely leads to a minimization of the batch time and hence increases the total throughput of the process unit.

Therefore a rational way of operating a batch crystalliser will be a trade-off between maximisation of throughput and achievement of sufficient product quality, provided by an upper limit on the crystal growth rate. From an industrial point of view (plant wide point of view) it is furthermore important that the batch will be ended in a stable operating condition (equilibrium), such that it can be intermediately stored before further processing in the downstream processing steps (e.g. filtering, drying).

As described above the control problem of a batch crystallisation process contains various requirements with different priorities, which can change in time. A batch crystalliser is a multi-variable system with non-linear, time-variant process dynamics. Constraints are

encountered on some of the process outputs, for instance the crystal growth rate, temperature in the crystalliser to guarantee production of the right polymorph, etc. Also on process inputs constraints may be specified, e.g. limited cooling capacity in cooling crystallisation and limitations on the heat-input for evaporative crystallisation. All these aspects make the control problem of a batch crystalliser well suited for a model predictive control approach [MAC02]. The MPC enables trade-offs between the different conflicting requirements, while ensuring that the specified process limitations are satisfied. A major difference with the average MPC problem is the large non-linear and dynamic operating range over which the process is excited during a batch. This calls for the application of non-linear MPC as presented in this paper.

2. Crystallisation Model

The cornerstone of a model predictive controller is its dynamic process model, describing the dynamic relation between the relevant inputs and outputs of the system to be controlled. The model is used both for prediction of the future behaviour of the dynamical system based on the plant's history (past) and the expected future inputs as well as for optimisation of the future process behaviour by adapting the future inputs based on a criterion function. In fact, model predictive control uses the model to continuously explore the degrees of freedom in the process to achieve maximum performance.

In standard application of model predictive control in industry, models are obtained by system identification. These models are based on historical process data obtained from tests applied to the process specifically for this purpose. This approach is not economically feasible anymore for systems which are operated over a large dynamic non-linear process range, such as batch crystallisation. Therefore, a physical modelling approach is necessary to make model predictive control feasible for batch crystallisation processes.

Batch crystallisation processes can be modelled by means of mass balances for each liquid (solvent and solute) and solid component, an energy balance and a population balance. Due to lack of detailed knowledge about the crystallisation phenomena taking place in crystallisation processes and for the sake of simplicity of the models needed for control, the crystallisation phenomena (e.g. growth and nucleation) are modelled by means of empirical relations (power law equations). The parameters of the empirical equations need to be estimated based on a set of historical data of normal batch operation and/or specific (limited) tests done on the batch crystallisation process.

The population balance equation is a hyperbolic partial differential equation whose solution is numerically obtained by discretisation of the crystal size distribution. These approaches convert the infinite dimensional distribution described by the partial differential equation into a finite number of ordinary differential equations. For an accurate solution of the population balance equation a large amount of discretisation points is required, which results in a large number of ordinary differential equations. For on-line control implementations a compact model is needed for an acceptable computational load (i.e. time required to obtain a solution). Further, the population balance approach leads to a highly complex model describing the crystal size distribution in great detail, which is not directly needed for control of the crystal growth rate of a batch crystalliser.

The method of moments can be used to transform the population balance equation into a finite low dimensional system. This method is an exact solution of the population balance equation, but reduces the level of detail in the sense that only properties of the total population are described and a detailed crystal size distribution is no longer available anymore. With the method of moments a batch crystalliser can be described in a compact way, which still contains the necessary information for control, namely the crystal growth rate and the crystal mass / crystal content within the batch crystallisation system.

The model of a batch crystalliser is a non-linear model of the following form:

$$\begin{aligned}\dot{x} &= f(t, x, u) \\ y &= g(t, x, u)\end{aligned}\quad (1)$$

in which f represents the model state equations, g the model output equations, x the state vector, u the vector of inputs, y the vector of outputs and t time.

The physical interpretations of the states are the moments of the crystal size distribution, the mass of each liquid component (solute concentration) and the total enthalpy of the system (temperature of the crystalliser). The input of the system is generally the mechanism to influence the supersaturation (e.g. cooling of the slurry, evaporation of the solvent).

Locally the non-linear model (Eq. 1) can be approximated by means of a linear model based on a first order Taylor expansion of the original non-linear model.

$$\begin{aligned}\dot{x} &= f(t^*, x^*, u^*) + \left. \frac{\partial f}{\partial x} \right|_{(t^*, x^*, u^*)} \Delta x + \left. \frac{\partial f}{\partial u} \right|_{(t^*, x^*, u^*)} \Delta u + \text{higher order terms} \\ y &= g(t^*, x^*, u^*) + \left. \frac{\partial g}{\partial x} \right|_{(t^*, x^*, u^*)} \Delta x + \left. \frac{\partial g}{\partial u} \right|_{(t^*, x^*, u^*)} \Delta u + \text{higher order terms}\end{aligned}\quad (2)$$

One way to determine the partial derivatives of the state and output equations of the dynamical system is numerical perturbation of all variables in the system.

Around the nominal operating point or at any point on the batch trajectory, $f(t^*, x^*, u^*)$ and $g(t^*, x^*, u^*)$, this model is equivalent to the following state space description:

$$\begin{aligned}\dot{x} &= Ax + Bu \\ y &= Cx + Du\end{aligned}\quad (3)$$

where the matrices A , B , C and D represent the above partial derivatives of the state and output equations with respect to the states and the inputs. The values of these matrices depend on the actual operating point. Hence, the time-variant batch operation of the non-linear batch crystallisation process makes these matrices highly time-variant.

3. The Model Predictive Control Architecture

The control architecture consists of an industrial model predictive control environment (INCA-NLMPC[®], IPCOS), an observer (Extended Kalman Filter (EKF) or Luenberger type) [KAL06], a non-linear moment model of a batch crystalliser and an OPC communication interface.

As can be seen in Figure 1 the software architecture used consists of different blocks each having their own specific task (controller, observer, data logging, data pre-processing, etc.). The internal communication as well as the communication between the framework and the real process (plant) is based on the OPC (OLE for Process Control) protocol, which has become the standard communication protocol used in process industry nowadays. The heart of the framework is an OPC server (IPCOS DataServer), containing all variables that have to be exchanged between the different tasks present in the architecture. At each sample moment a powerful scheduler determines which tasks to execute and in what order to execute them. The use of this architecture makes the framework very flexible. It is easily adaptable to the specific plant environment and to customer requirements. Moreover, the framework is completely open for third party and customer software.

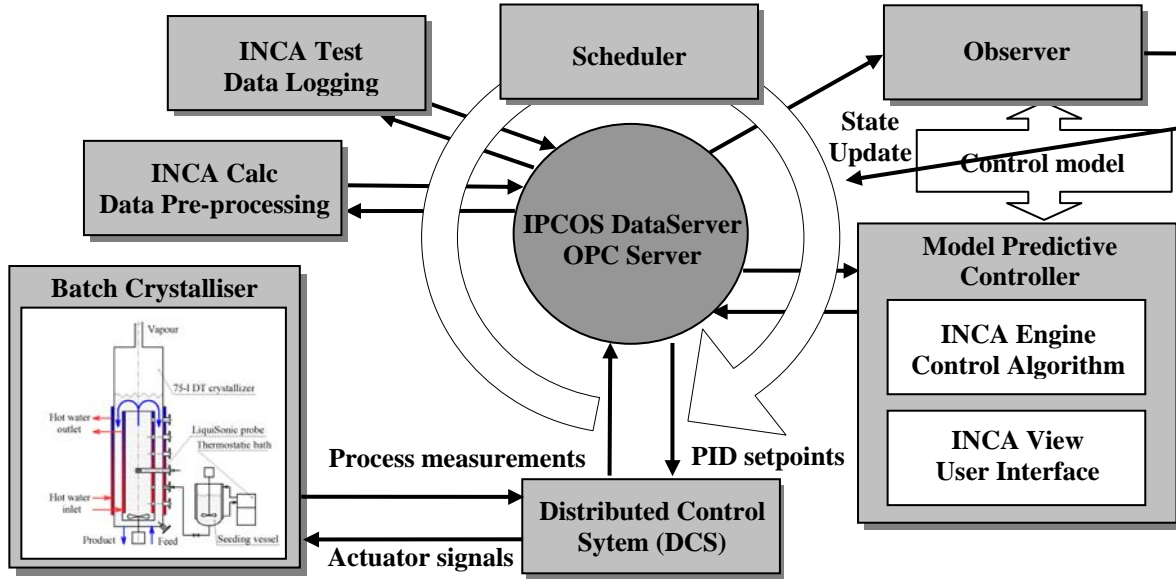


Figure 1. Block diagram of the Model Predictive Control architecture

Model Predictive Control (MPC) is an optimisation-based control strategy/algorithm. The model predictive controller uses a model together with on-line measurements of the relevant process variables to compute optimal control actions over a future horizon (the so-called control horizon N_c) given a certain objective function (evaluated over the so-called prediction horizon N_p) and constraints defined on the process inputs and outputs:

$$\min_{u_k, \dots, u_{k+N_c-1}} \sum_{i=1}^{N_c} \|u_{k+i} - u_{k+i}^{ref}\|_R^2 + \sum_{i=1}^{N_p} \|y_{k+i} - y_{k+i}^{ref}\|_Q^2 + \sum_{i=1}^{N_c} \|\Delta u_{k+i}\|_W^2 \quad (4)$$

Subject to:

$$u_{k+i}^{\min} \leq u_{k+i} \leq u_{k+i}^{\max}$$

$$\Delta u_{k+i}^{\min} \leq \Delta u_{k+i} \leq \Delta u_{k+i}^{\max}$$

$$y_{k+i}^{\min} \leq y_{k+i} \leq y_{k+i}^{\max}$$

with $\|z_i\|_W^2 = z_i^T W z_i$ and W is a symmetric definite matrix.

The objective is chosen such that it is possible to weigh deviations on the inputs/outputs with respect to their reference value (reference tracking) against control effort put into the system (punishment of the input moves Δu). The optimisation of this objective is subject to process limitations represented by absolute constraints on the process inputs/outputs and rate-of-change constraints on the inputs.

After solving the optimisation problem only the first value of the calculated future input sequences will be really implemented on the process. The next sample instant the optimisation is repeated based on new information gathered from the process. This principle is also known as the receding horizon principle [MAC02].

The MPC determines the optimal control actions in two steps: first an open-loop (without control) prediction of the system, followed by the optimisation of the above constrained criterion (Eq. 4). In the presented model predictive controller the prediction step is performed using the non-linear moment model of the batch crystallisation process. During the prediction a local Linear Time-Variant (LTV) model is extracted from the non-linear process model. This LTV model is then used in the second step, such that the optimisation is a quadratic problem with linear constraints (Quadratic Program - QP). In the next sample the

solution of the optimisation step is used as future input trajectory for the prediction step. The receding horizon implementation and the use of the previous solution as initial input trajectory in the next iteration makes the MPC optimisation step behave like a Sequential Quadratic Programming (SQP) over time.

The available process measurements (e.g. crystal content and CSD) are used by an observer to update the states of the process model used in the model predictive controller. This way, the model behaviour is prevented from diverging far from the plant's behaviour, induced by model mismatches, different initial conditions and unknown process disturbances. Additionally, process variables which cannot be directly measured online, such as crystal growth rate, can also be monitored by the updated process model (soft-sensing). Soft-sensing the crystal growth rate is necessary to incorporate the crystal growth rate as a quality constraint in the model predictive control algorithm.

4. Experimental Setup

The viability of the model predictive control framework for real-time applications is verified for a seeded fed-batch evaporative crystallisation of an ammonium sulphate-water system. The results of the experimental work are described in Section 6, while this section gives the overall process description. The framework is implemented on a semi-industrial 75-liter draft-tube crystalliser equipped with a Yokogawa Distributed Control System (DCS, CENTUM CS3000, Yokogawa, Japan). The well mixed crystalliser has one inlet and two outlet streams. The single inlet stream serves to keep the volume of the crystalliser constant by compensating for the losses in volume due to both evaporation of solvent at a constant temperature of 50°C and slurry sampling for CSD measurement. A vapor stream and an unclassified product removal stream on the other hand constitute the outlet flows. The CSD of the product is measured on-line by means of a laser diffraction instrument (HELOS-Vario, Sympatec, Germany). Samples are withdrawn from the crystalliser at regular time intervals and diluted with a saturated feed solution to reduce the volumetric crystal content. A thorough execution of sampling is crucial for obtaining reliable CSD measurement. The volumetric crystal content in the crystalliser is indirectly measured by a slurry density measurement, with the assumption of constant crystal and liquid density. The volumetric crystal content and the crystal size distribution are used together for on-line calculation of the moments of the crystal size distribution. This information is required by the applied Luenberger type of observer to keep the moment model in-line with the real process. The crystalliser is also equipped with an in-line concentration measuring probe (LiquiSonic 20, SensoTech, Germany) to measure the predetermined supersaturation level at which the ground seeds (600 g. of a size range of 90-125 µm) are inserted into the crystalliser vessel. The seed preparation procedure and the impact of seed sizes, seed loads and operating conditions on the product quality are discussed in [KAL07].

The outputs of the system to be controlled by the model predictive controller are the measured volumetric crystal content and the crystal growth rate. The crystal growth rate is an unmeasured variable, but it is estimated by the moment model. These outputs are called the Controlled Variables (CVs) of the model predictive controller. The input of the system is the heat-input, which is controlled by a Proportional-Integral (PI) controller of the DCS by changing the hot water flow through the wall- and draft-tube-mounted jacket of the crystalliser. The heat-input setpoint of this local PI controller is used as input, also called Manipulated Variable (MV), for the model predictive controller. It has a physical limitation of 13 kW, which is taken into account as a constraint in the controller. The already mentioned outlet flow used for sampling for the CSD measurement is taken into account in the model predictive controller as a Disturbance Variable (DV), which means that the controller takes the measured outlet flow into account in the prediction step (feed-forward control), but cannot influence the value of this variable.

5. Simulation Results

In this section simulation results are shown based on a moment model developed for the 75-liter draft-tube crystalliser described in Section 4. The model was validated based on data of several batches with different constant levels of heat-input. More details about the model, the model equations and its parameters can be found in [KAL06] and [MES08].

The presented control framework was applied to a plant simulator for which the same moment model was used as the one incorporated in the model predictive controller. No model mismatches between the plant model and the controller model are taken into account and the initial conditions (initial crystal size distribution, specified by the moments of the crystal size distribution, and the initial supersaturation level) of both models are identical.

In Figure 2 simulation results of three different experiments are shown: two reference experiments with constant levels of heat-input, respectively 9 kW (SIM1) and 4.5 kW (SIM2), and one experiment in which the model predictive controller was used and was allowed to manipulate the heat-input into the crystalliser (SIM3). The control problem of the presented model predictive controller was to produce as fast as possible 25 % of volumetric crystal content with an upper limitation on the crystal growth rate of 1.5 $\mu\text{m}/\text{min}$. Furthermore, the batch should be ended such that after ending the batch the crystal content remains constant; the batch is ended in a stable operating point.

The reference experiments show that by decreasing the heat-input from 9 to 4.5 kW the crystal growth rate is below the maximum value of 1.5 $\mu\text{m}/\text{min}$ during the entire batch. This comes however with a cost of a much lower production rate. After an equal amount of batch time the yield in crystal content of the 4.5 kW reference experiment is half that of the 9 kW experiment. By applying the model predictive controller it is possible to calculate on-line an optimal heat-input profile that keeps the crystal growth rate as high as possible throughout the batch. The controller really pushes the system to its limit. From SIM3 it can be seen that the controller also decreases the heat-input in the beginning of the batch to a value around 4.5 kW. At the moment that the crystal growth rate decays due to the increasing crystal content in the batch, the controller slowly increases the heat-input, while respecting the crystal growth rate constraint at 1.5 $\mu\text{m}/\text{min}$.

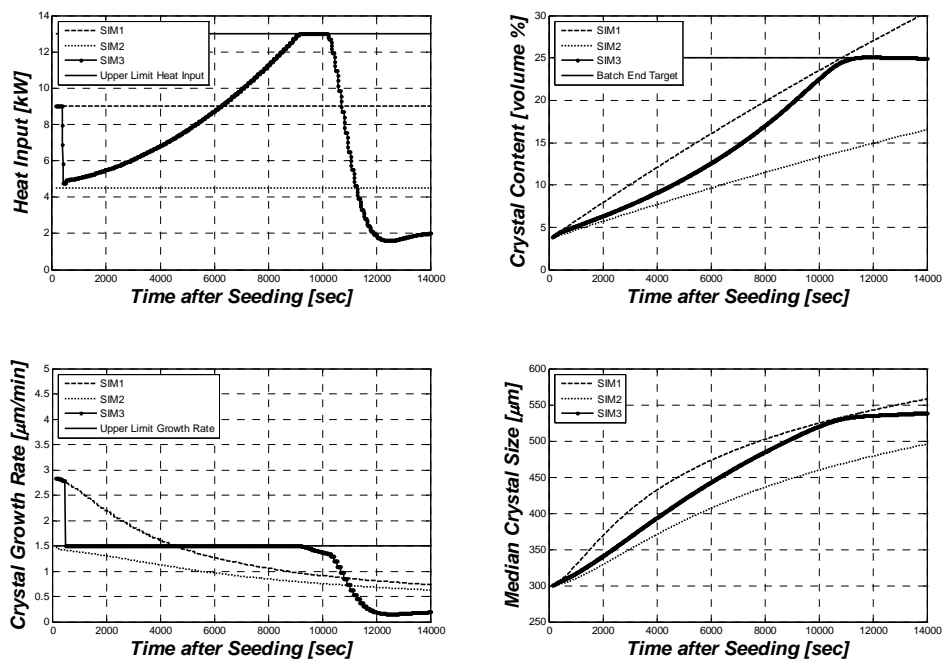


Figure 2. Simulation results of the applied Model Predictive Control architecture

At the end of the batch the controller stabilises the system at the final required volumetric crystal content of 25 % by reducing the heat-input such that the system “almost” comes to a steady state, namely at the conditions of a just saturated solution. The reason of writing “almost” is the fact that the system does not exactly stabilise with a heat-input of 0 kW. This is caused by the small unclassified product stream that makes the crystalliser loose some crystal material during the batch. In case of no outflow the controller would have controlled the process exactly to 0 kW of heat-input and saturated solution.

6. Experimental Results

Figure 3 shows the results of the experimental validation of the proposed model predictive control framework on the 75-liter draft-tube crystalliser at Delft University of Technology.

In the plots three different experiments are shown: one reference experiment without control (DTc31) and two experiments in which the model predictive controller was activated (DTc66 and DTc68). During the control experiments the controller was turned on after 3-5 correct CSD measurements were received from the laser diffraction instrument (taken each 2 minutes). This procedure was followed to ensure that the observer had updated the moment model properly and the controller got reasonable estimations of the crystal growth rate. All experiments were started with a heat-input of 9 kW.

During the reference experiment (DTc31) the heat-input was kept constant at 9 kW. As a result the crystal growth rate was initially above the maximum limit of 1.5 $\mu\text{m}/\text{min}$, but slowly decayed towards the end of the batch due to the increase of crystal mass. In the first 4000 seconds of the reference experiment the growth rate was high, which could have led to deterioration of the final product quality. After approximately 4000 seconds the growth rate dropped below the maximum limit. In this last part of the batch the growth rate is lower than the maximum value, which means there was still a possibility for increasing the production rate.

With experiment DTc66 it is shown that by means of manipulation of the heat-input the production rate could be maximised in the last part of the batch in such a way that the growth rate constraint is not violated. In DTc66 the initial growth rate was still above the

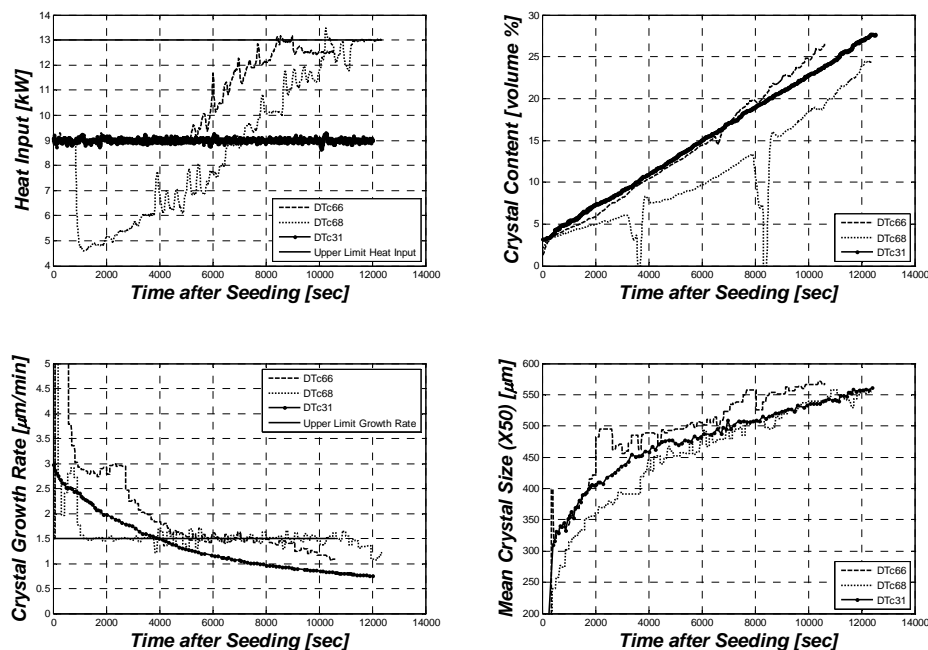


Figure 3. Experimental results of the applied Model Predictive Control architecture (the controller was activated at $t = 600$ seconds)

maximum limit, because a lower limit of 9 kW was put on the heat-input. The lower limit on the heat-input was implemented to insure the survival of the seed crystals that could possibly be dissolved in case of lower initial heat-input.

Experiment DTc68 shows that it is unlikely that decreasing the heat-input causes dissolution of the seeds. By removing the lower limit on the heat-input the controller was able to meet the requirement on the crystal growth rate during the entire batch. However, the lower crystal growth rate during the first part of the batch led to somewhat lower crystal content at the end of the batch compared to experiment DTc31. The drops in the crystal content measurement during experiment DTc68 were due to plugging in the sample line, which was solved by rinsing with water. The only part of the batch when the controller could not push the system towards its crystal growth rate constraint was the period during which the heat-input was touching its physical limitation of 13 kW. At that time the controller lost its degree of freedom and control was not possible anymore. The system then behaved like the reference experiment and the crystal growth rate slowly decayed due to the still increasing crystal content of the batch.

7. Concluding Remarks

In this paper an approach towards Model Predictive Control (MPC) of batch crystallisation is presented, with the objective of maximising the overall throughput of the batch crystallisation process without a loss of product quality. The quality requirement was implemented as an upper limit on the crystal growth rate, which should be satisfied during the complete batch.

Experimental results showed that as long as the process inputs were not constrained the controller was able to push the system against the upper limit specified for the crystal growth rate and in this way maximise the production of the unit operation.

Lowering the heat-input did not result in the expected improvement of product quality (CSD), probably because proper seeding resulted in process operation dominated by crystal growth and with limited nucleation. Furthermore, the maximum crystal growth rate was probably chosen in a conservative way (too low) and could be higher to increase the overall yield. The value chosen as the maximum crystal growth rate is somewhat arbitrary and based on experience with the system. In practice it could be adjusted in an inter-batch way, based on feedback of the Quality Assurance department. If the produced product is still within the quality specifications, probably the crystal growth rate can be increased to get more out of the system. On-line monitoring of the product quality, e.g. with video microscopy, could help in defining an optimal time-varying crystal growth rate constraint during batch operation.

8. References

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