Inferential control of a dextrose column crystallizer based on an Extended Kalman Filter

G. Bonadonna[1], M. Bravi[1,a], A. Chianese[1], T. Backx[2], W. Van Brempt[2]
[1]Department of Chemical Engineering, University of Rome "La Sapienza", Italy.
[2]IPCOS, Leuven, Belgium.
[a]m.bravi@ingchim.ing.uniroma1.it

The monitoring of the CSD of the crystal product from an industrial crystallizer requires measuring devices which are seldom applied. This difficulty may be overcome estimating the interesting variables by a soft sensor. The present work describes the application of an Extended Kalman filter for the estimation of the fines content in the crystal product of a continuous column crystallizer for the production of dextrose monohydrate and the subsequent development of an inferential control scheme of the crystallizer, by using the INCA control environment. A rigorous model of the crystallizer was used both to implement the EKF and to check the control process scheme performances.

1. Introduction

Although strictly connected with an important product quality specification, the monitoring of the CSD of the crystal product from an industrial crystallizer is still a troublesome operation. On-line and in-situ instruments, such as back scattering probes, are increasingly advocated for but they are very expensive and they measure chord length distributions (CLD) instead of crystal size distributions (CSD). In lack of a direct measurement of the crystal size characteristics (such as the percentage of fines) in the crystallizer outlet slurry, an estimate of the value of these variables can be obtained by means of an appropriate inference.
This work reports the application of an extended Kalman filter (EKF) for the estimation of the fines content in the crystal outlet slurry from a continuous column crystallizer for the production of dextrose monohydrate (DX). Firstly a simulation compartmental model of the crystallizer was developed by using the gPROMS package and a linear identification model was derived. This latter tool was then used to implement an EKF in the Matlab environment by using the EKO software package. After the tuning and validation of the EKF an inferential control scheme of the crystallizer was developed within the INCA control environment.

2. Reference Model Structure of the Adopted Crystallizer

The examined system is a dextrose monohydrate column crystallizer with a high capacity of several tens of m^3. The cooling system of this unit is made up by three series of geometrically identical cooling coils where water in counter-current flow arrangement is being used as the coolant. Stirring is provided by a multiple-blade impeller. A constant-flow rate of supersaturated dextrose solution with up to 10% of seeded crystals enters the crystallizer from the top of the unit, while the product slurry leaves it from a nozzle located at the bottom and is subsequently centrifuged to separate the solid crystal product from the suspending liquid. The crystallizer feed, in turn, results from the mixture of two streams, one being slurry with a high crystal concentration in a mother liquor with negligible supersaturation and another being an essentially crystal-free but highly supersaturated solution.
The process control variables are: 1. the magma density of the overall crystal slurry M_t

($Kg_{crystals}\ Kg_{suspension}^{-1}$), defined as $M_t \;=\; \frac{\rho_{crystal}}{\rho_{slurry}}\ {}_{L_{min}}^{L_{max}}\ K_v\ \ n\ L\ \ L^3 dL$; 2. The magma density of the crystals smaller than an adopted threshold size L_{fines} (here, 130 μm) M_{tf} ($Kg_{finecrystals}$ $Kg_{suspension}^{-1}$), defined as $M_{tf} \;=\; \frac{\rho_{crystal}}{\rho_{slurry}}\ {}_{L_{min}}^{L_{fines}}\ K_v\ \ n\ L\ \ L^3 dL$, representing one of the aspects of product quality. Although this latter parameter is the main process control variable, it is not normally directly measured.

The reference model structure of the adopted crystallizer is based on a compartmental approach. Following the structural subdivision determined by the three series of cooling coils, the crystallizer volume was split into 3 zones ("compartments") featuring homogeneous internal properties (i.e. null gradients) and different operating conditions (such as temperature) and process conditions (such as slurry density, CSD and physical properties, and solution supersaturation) between each other. Each compartment is described as a CSTR where the same balance, thermodynamic and kinetic equations apply. Moreover, each element of the compartment array is referenced by an upstream "frame" model representing the whole crystallizer.

The mass balance equations for the i-th component, i.e. DX and polysaccharides (PS) present in solution, and for the population for each compartment are:

$$V\ \rho\ \frac{d\ \ 1\text{-}Mt\ \ C_i}{dt} \;=\; Q\ \rho_{susp}\ \ 1\text{-}Mt_{in}\ \ C_{i,in}\ \ \ 1\text{-}Mt\ \ C_i$$

$$\frac{n\ L}{t} \;=\; \frac{n\ L\ G}{L} + \frac{n_{in}\ L\ \ Q_{in}}{V}\ \ \ \frac{n\ L\ \ Q}{V}$$

where C_i is mass fraction of DX or PS. In the implemented model it is assumed that nuclei are formed uniquely by catalytic mechanism. The boundary conditions of the differential equation are:

$$C_{i,in}\ \ \ C_{i,seed}$$

$$n_{i,in}\ \ \ n_{i,seed}$$

$$B_0\ \ \ n_0\ \ G$$

The growth rate of dextrose crystals is very low since it is affected by the polysaccharides as demonstrated by Parisi et al. [PAR03]. The growth rate expression used in this work is suggested by Terranova et al. [TER05]:

$$G\ L = K_0\ e^{\frac{E_a}{RT}}\ \sigma\ \ 1\ \ k_{nd}\ \ \frac{C_{PS}}{C_{PS}\ \ C_{DX}}$$

where for E_a, K_{nd} and K_o the values are 30.5 kJ $kmol^{-1}$, 1.5 and 3.2 m/h.

The adopted nucleation rate was suggested by Parisi et al. [PAR05]:

$$B_0\ \ \ \frac{0.607\ 10^7}{K_0}\ \ \ 3$$

3. The Estimator

In the reference crystallizer no provision is made for the continuous measurement of the magma density of fines; therefore, a state observer (i.e. an extension to a state space model used on a system where direct access to the state is not possible) was set up for this latter process variable based on the EKF.

While the classical Kalman filter was initially devised for the estimation of physical processes described by linear differential equations, it has been subsequently adapted ("Extended") to estimation tasks in non linear systems. The state-space description of a non linear system is:

$$X' = f(X, U, W)$$
$$Y \;\; g(Y, U, V)$$

where X, Y and U are the state, output and input vectors respectively, while W and V are the vectors of the noise affecting the state and controlled variables respectively.
The Kalman filter iterates through a "predictor" and a "corrector" step sequence, represented by two systems of difference equations. For the predictor step, the following applies:

$$\hat{X}_{k+1} = f\; \overline{X}_k, U_k, 0$$
$$\hat{Y}_{k+1} = g\; \hat{X}_{k+1}, U_k, 0$$

where $\hat{X}_{k+1}$ stands for the prediction of the $\overline{X}_K$ state carried out (and corrected) at time k, relevant to the $k+1$ discrete time, obtained assuming null values for the W and V noise vectors.
For the corrector step a less immediate calculation applies, requiring a linearization in Taylor series of the model equations; after doing this, keeping the first-order term and neglecting all higher order terms, the linearized model becomes:

$$X_k \;\; \hat{X}_k + A_k\; X_{k\,1} \;\; \overline{X}_{k\,1} \; + B_k\; U_{k\,1} \;\; \overline{U}_{k\,1} \; + B_k W_k$$
$$Y_k \;\; \hat{Y}_k + C_k\; X_k \;\; \hat{X}_k + D_k\; U_{k\,1} \;\; \hat{U}_{k\,1} \; + D_k V_k$$

where:

$$A_k\; i,j \;\; \frac{f_i\; \overline{X}_{k\,1}, U_{k\,1}, 0}{X_j} \qquad C_k\; i,j \;\; \frac{g\; \hat{X}_k, U_{k\,1}, 0}{X_j}$$

$$B_k\; i,j \;\; \frac{f_i\; \overline{X}_{k\,1}, U_{k\,1}, 0}{U_j} \;\; \frac{f_i\; \overline{X}_{k\,1}, U_{k\,1}, 0}{W_j} \qquad D_k\; i,j \;\; \frac{g\; \overline{X}_{k\,1}, U_{k\,1}, 0}{U_j} \;\; \frac{g\; \hat{X}_k, U_{k\,1}, 0}{V_j}$$

By applying a least-squares minimization on the above linearized system the equations for the calculation of covariance and of the "a posteriori" estimate can be derived:

$$\hat{P}_k = A\; \overline{P}_{k\,1}\; A^T + B\; Q\; B^T \qquad K = \frac{\hat{P}_k C^T}{R + C\hat{P}_k C^T}$$
$$\overline{X}_k = \hat{X}_k + K\;\; Y_k \;\; g\; \hat{X}_k, U_{k\,1} \qquad \overline{P}_k = 1 \;\; KC\,\hat{P}_k$$

The development of the observer was carried out with the aid of the EKO Engine package supplied by IPCOS executing in the Matlab (The Mathworks, USA) host environment. In the target application, a continuous, periodically corrected estimate of the magma density of fines is hereby made available to the subsequent controller element.
Prior to using the designed observer architecture in the target crystallizer control application it was tuned in order to attain an optimal performance according to the scheme reported in Figure 1. The gPROMS model was used both to simulate the process performances under disturbances and noises and the process prediction, while the EKF updated the state variables of the prediction model. The communication among the three packages was ensured by OPC (OLE for Process Control) channels and gateway provided by the INCA DataServer.

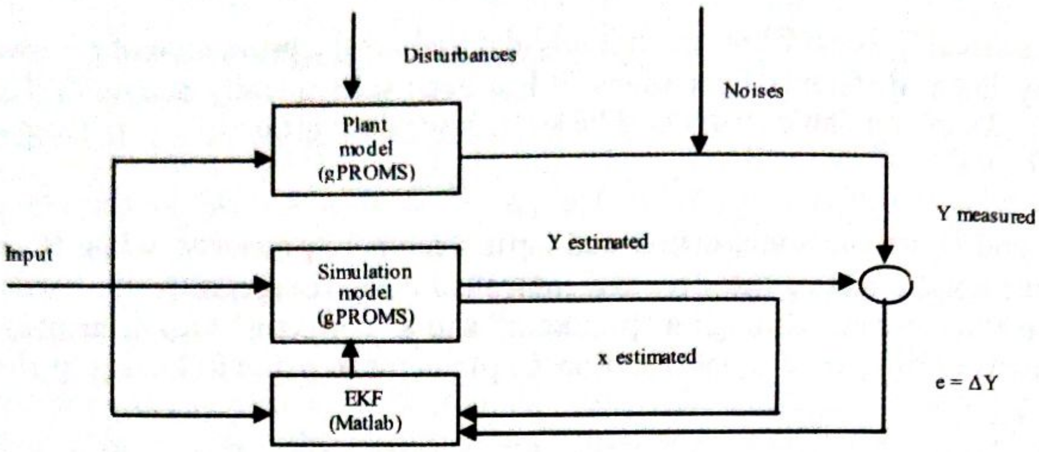


Figure 1. Scheme of the off-line system used to tune the EKF.

Initial sensitivity tests carried out on the process model provided suitable reference values for the operation and tuning of the EKF. In this implementation a 1-hour sampling time was adopted for all the measured variables; the choice of the sampling time is based on a trade-off between the filter prediction accuracy and the required computation time (which, for a large number of states, may either impose a lower bound on the sampling time or require a large computing power). The process input variables which do not change during the unit operation (namely, the cooling coils inlet temperature and the feed flow rate to the unit) were adopted as input variables in the EKF. The differential variables appearing in the balance equations of the crystallizer compartments were adopted as the filter states, while the crystallizer outlet stream concentrations and inlet and outlet temperature were adopted as the (continually) measured output variables.

The diagonal elements of the R matrix of the Kalman filter was populated with the measuring noise information, i.e. zero mean and standard deviation equal to 2% for concentration measurements and 0.5°C for temperature measurements.

A criterion was adopted to set up the state noise Q matrix, as the state values are not directly measurable; the initial value for this latter noise matrix was based on the standard deviations from the real process due to modeling errors, rather than the noise associated to a hypothetical measure.

The tuning of the filter was carried out considering a 10% variation in the amount of inlet crystals and a periodic (resulting from the sum of the output value and of a periodic measurement error) variation on the output variables which permitted to visually compare the obtained results in the time domain in different runs. Later, similar values were used during the filter validation stage.

The application of the EKF followed a two-stage pathway; while in the first stage constant process parameter values equal to the steady state values were adopted, in the second stage a 10% variation of the crystal mass content of the inlet slurry was included. In both stages random error components were added to the values of the output variables calculated by the process simulator with gaussian shape and zero mean and standard deviation equal to 4% of the average value for DX concentration and M_{tf} and 1°C for temperature.

The first EKF application stage was aimed at testing the error minimization capabilities of the filter in a steady state process condition. During this stage the standard deviation of the state noise was optimized with a trade-off between the information provided by the model and that provided by the measurements carried out in the model representing the crystallizer plant and receiving process disturbances (increased state noises lead to an estimator which makes a progressively lower confidence in the model). In order to appreciate the estimation capabilities increase of the filter, the test was repeated after the parameter tuning. Figures 2.a and 2.b show a significant damping in the errors after the filter tuning. The explanation to this behaviour is that in the former test the same weight is given to all the variables, while in the latter ones the weight is adjusted based on the sensitivity of each to the applied variation. The second EKF application stage was aimed at testing the error minimization capabilities of the filter in a typical dynamic process condition. The applied step disturbance in the inlet slurry concentration leads to a 5% variation in the magma density of fines, while none of the other monitored process variables varies significantly. Figure 2.c compares the EKF prediction to the output of the measurement error-free simulation model; the slight offset in the prediction is a function of the EKF operation sampling time.

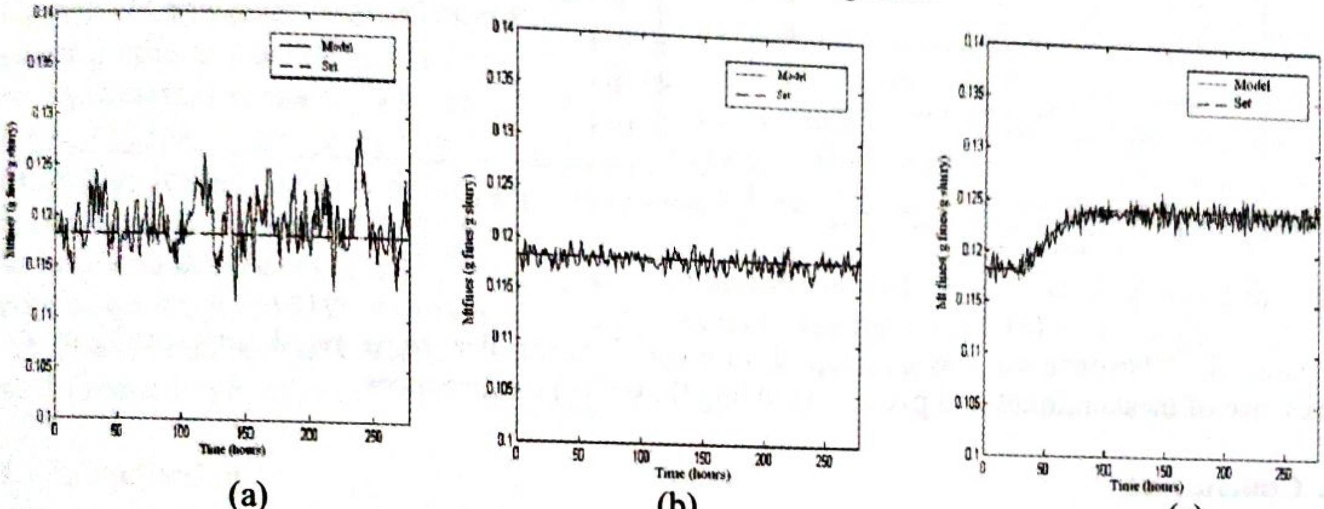


Figure 2. Effect of tuning on fines magma density.

4. Inferential Control of the Continuous Crystallizer

Based on the developed and optimized state observer an inferential scheme control of the product magma density of fines was developed with the aid of the gPROMS package (Fig. 3). The controller acquired a continuous estimate of M_{Tf} from the EKF; this latter, in turn, was periodically corrected by "sampling" the M_{Tf} value calculated by the model representing the process such as, in real life, the EKF estimate would be periodically corrected by off-line fines measurements by process turbidimetry. The adopted controller is of the PI type and is aimed at controlling the outlet magma density of fines by manipulating the amount of seeding in the feed (hence the overall magma density of the feed).

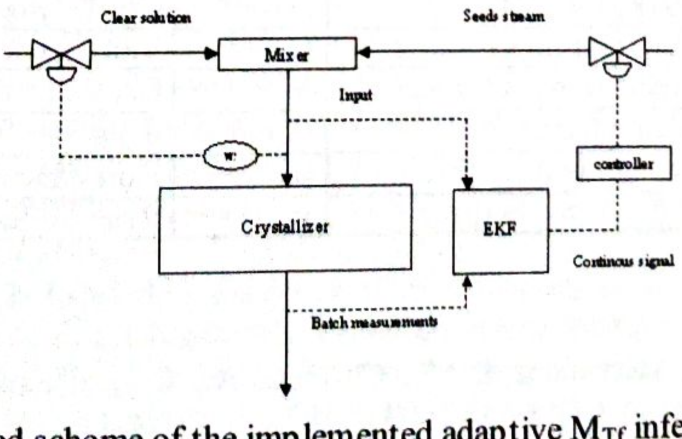
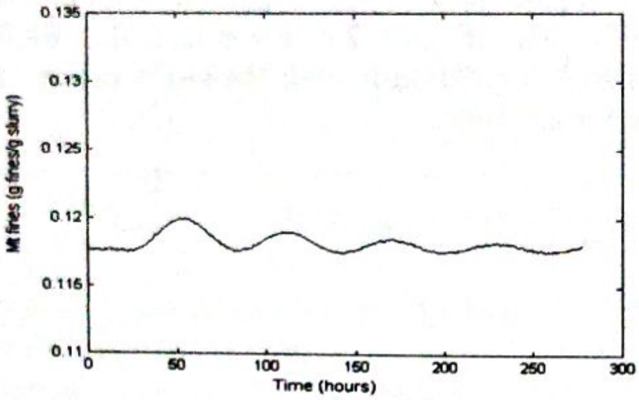
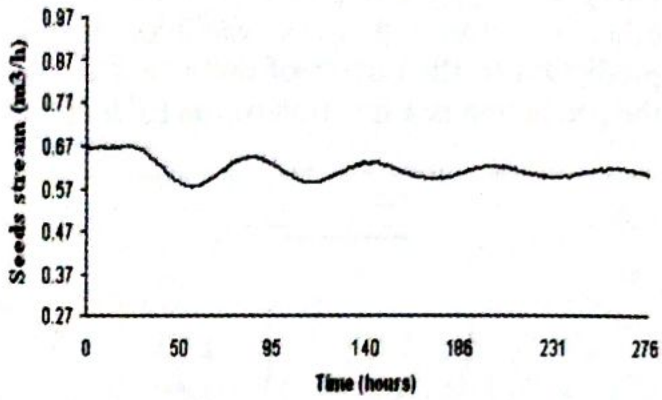


Figure 3. Simplified scheme of the implemented adaptive M_{Tf} inferential controller

The inferential control scheme was checked in regulatory-type problems, relevant to a disturbance in the crystallizer internal slurry density (10% of the steady state value). The time history of the controlled and manipulated variables following the onset of the disturbance action is shown in Figures 4a and 4b, respectively. It can be seen that, although the reaction curve exhibits a prolonged oscillation extending over several residence times of the crystallizer, the deviation of the magma density of fines remains within a tight interval and poses no practical problems in actual plant management.





(a) (b)

Figures 4. Response of the developed inferential controller to a regulatory problem in presence of measurement and process (seeding flow rate) disturbances.

5. Conclusions

Most operating crystallizers are poorly equipped from the point of view of CSD measurement and control, with the consequence that the control of CSD in the crystal product is more a matter of operator's experience and capability of coping with the outlet product of the crystallizer with the aid of downstream processing equipment than actual capability of determining it by means of adequate control actions.

In the presented work an inferential estimator of the magma density of fines in the outlet stream of a continuous industrial-size dextrose crystallizer based on the Extended Kalman Filter was developed and tuned. Furthermore, a PI inferential control strategy of the magma density of fines was set up and successfully tested in some cases of practical relevance.

6. Nomendature

C	Mass fraction (kg/kg sol.)	n(L)	Crystal population density (#/m^3·m)
G	Crystals growth rate (m/h)	Q	Volumetric flow rate (m^3/h)
K_{nd}	Growth rate reduction coefficient	V	Crystallizer volume (m^3)
K_v	Volumetric shape factor	Greek symbols	
K_0	Growth rate coefficient (m/h)	ρ	Slurry Density (Kg/m^3)
L	Crystal second dimension (μm)	σ	Relative Supersaturation

7. References

[PAR03] Parisi M., Hernandez I. M., Chianese A., Crystallization kinetic of Dextrose monohydrated, CGOM-6, 2003

[PAR05] Parisi M., Rivallin M., Chianese A., Prediction of the dextrose nucleation kinetics by the growth rate of crystallites, ISIC16, Dresden, 2005

[TER05] Terranova A., Parisi M., Chianese A., Bonadonna G., Modelling and optimal kinetics parameters set estimation for a batch crystallizer, ISIC16, Dresden, 2005