

Prediction-based delay compensation for staged crystallization

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Prediction-based delay compensation for staged crystallization

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1 Introduction

Traditionally, the crystallization of active pharmaceutical ingredients (API) and other chemical specialties has been operated in batch or semi-batch mode under strictly regulated recipes. However, batch operations have disadvantages such as lack of batch to batch reproducibility, long processing times, scale up issues, poor controllability and observability [1]. Continuous operation can overcome these drawbacks, although a higher degree of automation and a more in depth process understanding is required for successful continuous API production. Therefore, recent research efforts are directed towards the design of continuous crystallization processes. Multistage mixed suspension mixed product removal (MSMPR) crystallization might be the most convenient route of transition from batch to continuous operation, since current crystallizers in industry are of the stirred tank type [2]. Majority of the work in this area has studied the steady state properties of these systems whereas only a few works deal with the process dynamics and control of these units. In this work, an advanced control scheme for average crystal dimension control in industrial-scale two stage MSMPR crystallizers is proposed and tested in simulation.

2 Control problem

The particle size distribution (PSD) is an important property of a crystalline product. It can determine the efficiency of the downstream operations, as well as end-use properties, such as bioavailability. The control of the full PSD is not possible in practice. However, some of its attributes (average size, coefficient of variation, fines fraction, etc.) can be controlled. The scope of this work is to achieve the control of the average crystal length d_{43} . To this end, we opted for a control scheme that combines feedback control with process predictions. This is an effective and simple way to upgrade low level PI controllers to the level of advanced process controllers (APCs) that should not require highly skilled personnel for controller commissioning and maintenance [3].

3 Prediction-based time delay compensator

The core of the control scheme is presented in Fig. 1, and consists of a PI controller ($d_{43}C$ block) which manipulates the temperature setpoint in the first crystallizer jacket (T_1^{SP}) such that the average crystal length d_{43} is maintained at the desired specification. Because of the large volumes involved

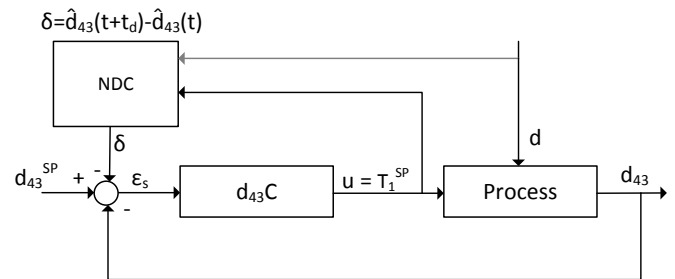


Figure 1: Block diagram of the advanced d_{43} controller. The block $d_{43}C$ is the linear PI controller with modified error signal ϵ_s ; the block NDC is the nonlinear delay compensator which can incorporate exogenous disturbance measurements d .

in the industrial operation, a large time delay t_d between manipulated and controlled variables can exist, resulting in limitations in the performance of this standard PI controller. Hence, a delay compensator is designed to improve closed loop performance by taking into account an additional error signal for future $d_{43}(t+t_d)$ deviations. The delay compensation block (NDC in Fig. 1) for average crystal length prediction consists of the nonlinear dynamic model of the first five PSD moments, solute concentration and temperature in the two crystallizers, with simulation horizon equal to the time delay. Measured disturbances, if available, can be provided to this model-based block for further performance improvements. A good control performance indicator is the ITAE which, in this case, is reduced at least by a factor of 4 by upgrading the PI controller with the NDC.

4 Acknowledgements

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