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Real-time feasible multi-objective optimization based nonlinear model predictive control of particle size and shape in a batch crystallization process

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A B S T R A C T

This paper presents nonlinear model predictive control (NMPC) and nonlinear moving horizon estimation (MHE) formulations for controlling the crystal size and shape distribution in a batch crystallization process. MHE is used to estimate unknown states and parameters prior to solving the NMPC problem. Combining these two formulations for a batch process, we obtain an expanding horizon estimation problem and a shrinking horizon model predictive control problem. The batch process has been modeled as a system of differential algebraic equations (DAEs) derived using the population balance model (PBM) and the method of moments. Therefore, the MHE and NMPC formulations lead to DAE-constrained optimization problems that are solved by discretizing the system using Radau collocation on finite elements and optimizing the resulting algebraic nonlinear problem using Ipopt. The performance of the NMPC–MHE approach is analyzed in terms of setpoint change, system noise, and model/plant mismatch, and it is shown to provide better setpoint tracking than an open-loop optimal control strategy. Furthermore, the combined solution time for the MHE and the NMPC formulations is well within the sampling interval, allowing for real world application of the control strategy.

1. Introduction

Batch crystallization is a crucial process in the pharmaceutical industry because more than 90% of the active pharmaceutical ingredients (API) are in the form of crystals (Alvarez & Myerson, 2010). The crystal size and shape distribution is of great concern to both product quality and downstream processing such as filtration. Therefore, the goal of batch crystallization is to control the crystal qualities to achieve the desired size and shape distribution at the end of the batch process. Primarily because of the technology limitations to monitor the crystal shape (Nagy, Fevotte, Kramer, & Simon, 2013), early works in the crystallization research community focused on modeling and controlling the size distribution of crystals (Mesbah, Kramer, Huesman, & Van den Hof, 2009; Qamar, Mukhtar, Seidel-Morgenstern, & Elsner, 2009). Focused Beam Reflectance Measurements (FBRM) is frequently used to monitor the size distribution online (Braatz, 2002; Fujiwara, Nagy, Chew, & Braatz, 2005; Puel, Févotte, & Klein, 2003). The last decade has witnessed a significant progress in monitoring and modeling the shape distribution of crystals allowing the standard feedback control (Mesbah, Huesman, Kramer, Nagy, & Van den Hof, 2011; Mesbah, Nagy, Huesman, Kramer, & Van den Hof, 2012; Nagy & Braatz, 2003; Patience & Rawlings, 2001; Wan, Wang, & Ma, 2009; Wang, De Anda, & Roberts, 2007). Derived using the multidimensional population balance model (PBM) (Hulburt & Katz, 1964; Ramkrishna, 2000) and the method of moments, the dynamic evolution of the crystal size and shape distribution can be modeled as a system of differential algebraic equations. The size and shape distribution can be controlled by manipulating the cooling profile of the reactor, which directly affects the supersaturation.

To balance the trade-off between the size and shape distribution, Acevedo, Tandy, and Nagy (2015) proposes a multi-objective optimization approach to control both the size and shape distribution offline. However, in the presence of model/plant mismatch and system noise, the real plant trajectory can be quite different from the optimal trajectory obtained from the open-loop multi-objective optimization. Therefore, in this paper, we developed a nonlinear model predictive control (NMPC) formulation that can be used to control the crystal size and shape distribution in real-time and in the presence of modeling and measurement noise.

Linear MPC has been a popular advanced control strategy in industry for many years (Qin & Badgwell, 2003). Because of the advances in both computational power and optimization algorithms, nonlinear model predictive control (NMPC) has become more computational feasible and is more appropriate for inherently nonlinear systems to achieve higher product quality and satisfy tighter regulations (Mayne, Rawlings, Rao, & Scokaert, 2000; Rawlings, 2000). The basic idea of NMPC is to solve an optimal control problem at each sampling instance with

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the updated measured or estimated states. The control values for only the next sampling instance are implemented and the entire process is repeated in the next sampling cycle. For batch processes, since our real interest is in the product quality at the end of the batch, end-point based shrinking horizon NMPC formulation is frequently used.

Nevertheless, for many processes, it is not possible (or cost effective) to accurately measure all states online, and model parameters may change from batch to batch. This challenge drives the need for a state estimator to reconstruct unknown states and parameters. The Extended Kalman filter (EKF) is a popular state estimator for unconstrained systems (Prasad, Schley, Russo, & Bequette, 2002). However, this technique is not appropriate for the batch crystallization model because of the highly nonlinear dynamics and hard constraints such as nonnegative concentrations. In contrast, nonlinear moving horizon estimation (MHE) uses nonlinear constrained optimization to estimate unknown states and parameters and has proven its advantages over EKF in many applications (Haseltine & Rawlings, 2005; Rao, Rawlings, & Mayne, 2003; Rawlings & Bakshi, 2006). Therefore, in this work, we propose an MHE formulation that can be used to estimate the unmeasured states in our model prior to solving the NMPC problem for the batch crystallization process.

The computational burden of this approach is that at each sampling instance, an expanding horizon estimation problem and a shrinking horizon model predictive control problem need to be solved. Both problems are DAE-constrained optimization problems and there exist multiple solution approaches. "Optimize then discretize" or indirect approaches try to solve the first-order optimality conditions for the DAE-constrained problem. For problems without inequality constraints, the first-order optimality conditions can be formulated as boundary value DAE problems. However, for problems with active inequality constraints, determining the switch points of the inequality constraints can become very challenging and thus limits the application of these methods. On the contrary, "discretize then optimize" or direct approaches discretize the control variables and solve the resulting nonlinear programming (NLP) problems. Among "discretize then optimize" approaches, the sequential approach discretizes only the control variables and treats the DAE system as a black box. A DAE integrator is used to simulate the system at each iteration and calculate its sensitivity with regards to the discretized control variables. One drawback of this approach is that the solution time increases significantly when the controls are discretized finer. However, a finer discretization of the controls can often improve the performance of the NMPC. In contrast, the simultaneous approach (Biegler, 2007; Biegler, Cervantes, & Wächter, 2002) discretizes both control and state variables and optimizes the resulting algebraic nonlinear problem with an NLP solver. The performance of the simultaneous approach is less dependent on the number of discretized control variables. Another advantage of this approach is that state constraints can be formulated in a more straightforward way. Therefore, this paper chooses the simultaneous approach to solve these DAE-constrained optimization problems arising from the NMPC–MHE formulations. One challenge of using the simultaneous approach is that the burden of manually discretizing the DAE system before it is embedded into an optimization formulation often lies on the user. However, packages such as the Modelica-based JModelica.org platform (Åkesson, Årzén, Gäfvert, Bergdahl, & Tummescheit, 2010) allow for straightforward declaration of differential equations and automatically perform this transcription process. Therefore, we implement these control formulations for batch crystallization within the Modelica library, which is already interfaced with solvers like Ipopt. If Ipopt is not fast enough, some parallel solvers can potential be used (Cao, Laird, & Zavala, 2016; Cao, Seth, & Laird, 2016; Kang, Cao, Word, & Laird, 2014).

This paper is organized as follows: a description of the unseeded batch crystallization model is presented in Section 2. Section 3 presents the NMPC–MHE approaches and efficient methods to solve the related optimization problems. Section 4 demonstrates the performance of the NMPC–MHE compared with the open-loop control in terms of setpoint change, system noise, and model/plant mismatch. Final conclusions are presented in Section 5.

2. Multidimensional unseeded batch crystallization model

This section provides a brief description of the multidimensional unseeded batch crystallization model. The details can be found in Acevedo and Nagy (2014). The population balance model (PBM) has been widely used to describe the crystallization process (Cao, Kang, Nagy, & Laird, 2016; Mesbah et al., 2012). Considering only the effect of growth and nucleation, the population balance equation for a well-mixed batch crystallization process can be expressed as

$$\frac{\partial}{\partial t}n(t,X)+\nabla_X[Gn(t,X)]=B\delta(X-X_0) \tag{1a}$$

$$n(0,X)=n_0(X), \tag{1b}$$

where $n(t,X)$ is the density distribution at time t, X is the vector of characteristic lengths, G is the vector of growth rates, B is the nucleation rate, X_0 is the size of the nuclei, δ is the Dirac delta function acting at $X=X_0$, and $n_0(X)$ is the initial seed distribution. The population balance model can be transformed into a set of ordinary differential equations (ODEs) using the method of moments (MOM). If we only consider two characteristic dimensions, the length L and the width W of crystals, the moments can be expressed by

$$\mu_{ij}=\int_0^\infty\int_0^\infty n(t,X)W^iL^j\,dW\,dL. \tag{2a}$$

The ODEs obtained from the MOM with the assumption that the nucleus size is negligible, are given by

$$\frac{d\mu_{00}}{dt}=B \tag{3a}$$

$$\frac{d\mu_{10}}{dt}=G_1\mu_{00} \tag{3b}$$

$$\frac{d\mu_{01}}{dt}=G_2\mu_{00} \tag{3c}$$

$$\frac{d\mu_{11}}{dt}=G_1\mu_{01}+G_2\mu_{10} \tag{3d}$$

$$\frac{d\mu_{20}}{dt}=2G_1\mu_{10}, \tag{3e}$$

where G_1 and G_2 are the growth rates along the width and length of the crystals respectively, and B is the nucleation rate. In this work, size independent growth rates and primary nucleation rate are considered as follows:

$$G_1=k_{g_1}S^{g_1} \tag{4a}$$

$$G_2=k_{g_2}S^{g_2} \tag{4b}$$

$$B=k_bS^b \tag{4c}$$

$$S=\frac{C-C_s(T)}{C_s(T)}, \tag{4d}$$

where the kinetic parameters $k_{g_1}, k_{g_2}, g_1, g_2, k_b$, and b are usually sensitive to process conditions. S is the relative supersaturation, C is the solute concentration, and C_s is the equilibrium concentration at a given temperature, which can be expressed using a polynomial expression, given by

$$C_s(T)=cT^2+dT+e. \tag{5a}$$

According to the mass balance equation, the evolution of the solute concentrate is given by

$$\frac{dC}{dt}=-2\rho_ck_vG_1(\mu_{11}-\mu_{20})-\rho_ck_vG_2\mu_{20}, \tag{6a}$$

where ρ_c is the density of the solution and k_v is a constant volumetric shape factor.

3. Computationally efficient online NMPC–MHE

At the end of the batch crystallization process, the product qualities are evaluated in terms of the size and shape distribution of crystals. Therefore, the mean length (ML) and aspect ratio (AR) are used to