Available online at www.sciencedirect.com

ScienceDirect

IFAC-PapersOnLine 49-7 (2016) 037–042

A robust NMPC scheme for semi-batch polymerization reactors

Hong Jang*, Jay H. Lee*, Lorenz T. Biegler**

** Department of Biomolecular and Chemical Engineering, Korea Advanced Institute of Science and Technology, 291 Daehak-ro, Yuseong-gu, Daejeon, 34141, Republic of Korea (e-mail: crimson1001@kaist.ac.kr)*
*** Chemical Engineering Department, Carnegie Mellon University, Pittsburgh, PA 15213, USA (e-mail: biegler@cmu.edu)*

Abstract: A robust nonlinear model predictive control (NMPC) scheme is proposed for batch processes with multiple types of uncertainties. Recently, economic MPC (eMPC) has attracted significant attention, particularly for batch process control given its flexibility in the cost function while addressing the nonlinear constrained multivariable dynamics seen in most batch processes. However, in the presence of various uncertainties such as parameter errors, external disturbances, and noise, performance of eMPC can deteriorate significantly as it tends to drive the system to limits of constraints. To achieve constraint satisfaction in the presence of common uncertainties, we propose a robust NMPC method based on multi-stage scenarios, state estimation, and back-off constraints. Performance of the proposed robust NMPC scheme is evaluated through an example of anionic propylene oxide polymerization reactor.

Keywords: Robust nonlinear model predictive control; Stochastic programming; State estimation; Back-off constraint; Batch process; Polymerization reactor

1. INTRODUCTION

Batch (or semi-batch) processes are widespread in the chemical process industry for producing low-volume, high value-added products, including polymers and specialty chemicals. Batch processes pose some inherent challenges brought by 1) transient operation and strongly nonlinear process dynamics, 2) presence of both path and end-point constraints, and 3) insufficient intra-batch measurements, esp. on product quality. Most batch operations are based on executing fixed, conservative recipes with some minor adjustments from batch to batch.

In this context, process control research has mostly focused on the problem of executing a given recipe in a precise manner, *e.g.,* following pre-specified reference trajectories using concepts like iterative learning control (ILC) to achieve batch-to-batch improvements in the tracking performance (J. H. Lee & Lee, 2007). In addition, batch-to-batch recipe adjustments have been studied to satisfy end product quality specifications in the presence of repeating errors, particularly in the context of processes in semiconductor manufacturing, using various run-to-run control techniques (Wang, Gao, & Doyle, 2009). Model based control techniques that combine real-time feedback control and ILC have also been proposed (K. S. Lee, Chin, Lee, & Lee, 1999), which were later extended to include end product quality control by further incorporating the concepts of run-to-run control and inferential control (Chin, Lee, & Lee, 2000). A number of researchers have studied the application of nonlinear model predictive control (NMPC) to batch processes, so that nonlinear constrained multivariable dynamics of batch processes can be addressed explicitly (Russell, Robertson, Lee, & Ogunnaike, 1998).

Increased competition has forced the chemical industry to consider real-time optimization (RTO) to enhance profitability while meeting various product/process constraints. Improvements in computing hardware and mathematical programming have made the use of optimization based on a detailed, rigorous first-principles model feasible and industrial applications have begun appearing. For example, model-based optimization has been used to improve the operating recipe of a semi-batch polymerization reactor, *e.g.,* to minimize the batch processing time while satisfying the constraints for product quality and process safety (Nie, Biegler, Villa, & Wassick, 2013). More recently, RTO has been developed for the same polymerization reactor using economic MPC (eMPC) (Jung, Nie, Lee, & Biegler, 2015). eMPC uses a more general cost function (e.g. minimizing batch time) that represents the process economics rather than the tracking error (Idris & Engell, 2012).

In general, various types of uncertainties exist for industrial batch processes; these can be largely classified into three types: parameter errors, external disturbances and noises. Parameter errors include mismatched values in kinetic parameters, mass/heat transfer coefficients, etc. External disturbances include variations in the utility conditions and feed conditions, which manifest as state initialization errors. Noises include measurement noises in sensing devices. In the presence of these uncertainties, performance of eMPC can deteriorate significantly. One important feature of eMPC is that it typically drives the system to an intersection of its constraints (Lucia, Andersson, Brandt, Diehl, & Engell, 2014). This, together with various uncertainties, can lead to severe violations of constraints, which can adversely impact product quality and process safety.

The issue of uncertainty has been studied extensively by the robust control community and within the specific context of MPC as well. Initial literature on the latter adopted an open-loop min-max formulation, which calculates control inputs that minimize the worst-case cost with respect to the defined bounded set of parameters (Campo & Morari, 1987). This

10.1016/j.ifacol.2016.07.213

approach, however, turned out to be not only conservative but also not robust due to the mismatch between the open-loop control assumption and the actual closed-loop implementation. To overcome this problem, closed-loop min-max formulations have been studied, but with limited success due to the inherent computational complexity (J. H. Lee & Yu, 1997). Tube-based MPC was proposed as an alternative, which uses an ancillary controller to ensure that the real uncertain system stays within a tube (Mayne, Kerrigan, Van Wyk, & Falugi, 2011). It can guarantee stability and constraint satisfaction in the presence of uncertainties, but does not address the issue of optimal performance. Recently, multi-stage NMPC has been suggested based on the idea of scenario branching and stochastic programming (Lucia, Finkler, & Engell, 2013). In this scheme, uncertainties are modeled using a scenario tree and the future control inputs are optimized as recourse variables to reduce the conservativeness of the solution.

In this paper, we propose a robust NMPC scheme based on multi-stage NMPC (or multi-stage eMPC) with additional features to deal with multiple types of uncertainties. It is an extended version of our previous work, which considered the constraint satisfaction against noise using a back-off approach (Jung, et al., 2015). Multi-stage NMPC is adopted to guarantee the constraint satisfaction in the presence of modeled parameter errors. Batch least-squares estimation (LSE) method is implemented for estimating the uncertain parameters and states while filtering the measurement noise. In addition to this, the back-off approach is used to account for noises, which are not handled by the batch LSE. Performance of the proposed scheme is evaluated through an example of a large-scale anionic polymerization of propylene oxide (PO) process with end product specifications and safety constraints.

2. ROBUST NMPC SCHEME

In this paper, a robust NMPC scheme for batch (or semi-batch) processes is proposed as described in Fig. 1.

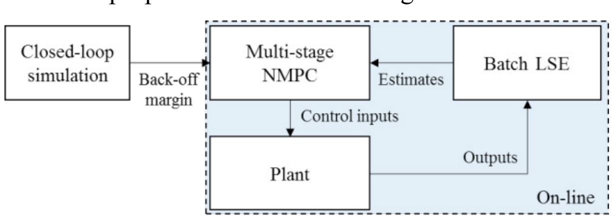

Fig. 1. A framework of robust NMPC scheme for batch processes

During each batch run, multi-stage NMPC calculates the control inputs at each time to minimize the batch time and satisfy the path and end-point constraints given the state and parameter estimates from batch LSE. The back-off margins obtained from closed-loop simulations with a given controller and expected uncertainties are introduced to tighten the constraints. NMPC uses a shrinking horizon (spanning from the current time to the final time) while LSE uses an expanding horizon (from the starting time to current time).

The multi-stage NMPC and batch LSE problems are converted to nonlinear programming (NLP) problems using the simultaneous collocation approach with uniform finite elements. This approach offers several advantages over the sequential approach in terms of treating nonlinear dynamics as well as path constraints (Biegler, 2010). The control inputs are assumed to be held constant within each finite element, while the state variables are further discretized using the orthogonal collocation points.

2.1. Multi-stage NMPC

Multi-stage NMPC generates a scenario tree, the branches of which represent the possible progressions of deterministic parameter errors, as shown in Fig. 2.

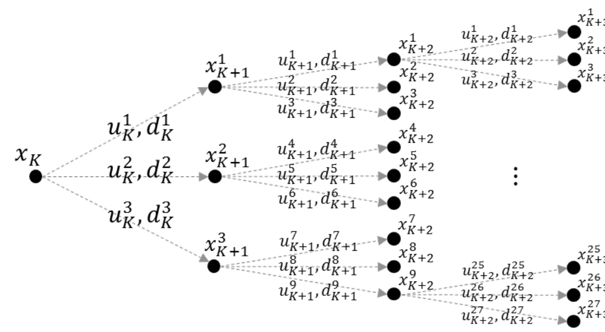

Fig. 2. A representation of scenario tree for multi-stage NMPC at the current stage K

A notable feature of this stochastic programming formulation is that the future control inputs are optimized as recourse variables that can take different values based on the realized scenario. This reduces the conservativeness of the solution. All control inputs that branch from the same node are set equal because the uncertainties that branch from that node are unknown, but are assumed to be resolved at the next stage, so that a branch is enabled to the next stage. These so-called non-anticipativity constraints are shown below in (11).

The multi-stage NMPC is formulated as

$$\min_{x_{k+1}^j, u_k^j, k=K,\dots,N_T-1, j=1,\dots,N_S(k)} \sum_{k=K}^{N_T-1} \left\{ \sum_{j=1}^{N_S(k)} \frac{\mathcal{L}(x_{k+1}^j, u_k^j)}{N_S(k)} \right\} \tag{1}$$

where x_k^j is the state (column) vector, u_k^j is the input (column) vector, j is the scenario index with $j = 1, \dots, N_S(k)$, k is the time (or stage) index with $k = K, \dots, N_T$, and K is the current stage. Note that, in Fig. 2, $N_S(K) = 3$, $N_S(K+1) = 9$, $N_S(K+2) = 27$, etc. $\mathcal{L}(x_{k+1}^j, u_k^j)$ is the stage-wise cost of the kth stage for the jth scenario defined by,

$$\mathcal{L}(x_{k+1}^j, u_k^j) = \Delta t_b + \mu P \tag{2}$$

$$\Delta t_b = t_{N_k} - t_K \tag{3}$$

Constraints are given as,

$$x_{k+1}^j = f\left(x_k^{p(j)}, u_k^j, d_k^j\right) \tag{4}$$

$$g(x_k^j, u_k^j) = 0 \tag{5}$$

$$c_p(x_k^j, u_k^j) \le 0 \tag{6}$$

$$c_e(x_{N_T}^j, u_{N_T-1}^j) \le P, P \ge 0 \tag{7}$$