Computers and Chemical Engineering 108 (2018) 47–56

Contents lists available at ScienceDirect

Computers and Chemical Engineering

journal homepage: www.elsevier.com/locate/compchemeng

Full length article

NMPC using Pontryagin's Minimum Principle-Application to a two-phase semi-batch hydroformylation reactor under uncertainty

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A R T I C L E I N F O

Article history:
Received 23 April 2017
Received in revised form 18 August 2017
Accepted 19 August 2017
Available online 26 August 2017

Keywords:
Nonlinear model predictive control
Indirect optimization methods
Indirect adjoining
Semi-batch processes
Pontryagin's Minimum Principle

A B S T R A C T

Nonlinear model predictive control (NMPC) is an important tool for the real-time optimization of batch and semi-batch processes. Direct methods are often the methods of choice to solve the corresponding optimal control problems, in particular for large-scale problems. However, the matrix factorizations associated with large prediction horizons can be computationally demanding. In contrast, indirect methods can be competitive for smaller-scale problems. Furthermore, the interplay between states and co-states in the context of Pontryagin's Minimum Principle (PMP) might turn out to be computationally quite efficient.

This work proposes to use an indirect solution technique in the context of shrinking-horizon NMPC. In particular, the technique deals with path constraints via indirect adjoining, which allows meeting active path constraints explicitly at each iteration. Uncertainties are handled by the introduction of time-varying backoff terms for the path constraints. The resulting NMPC algorithm is applied to a two-phase semi-batch reactor for the hydroformylation of 1-dodecene in the presence of uncertainty, and its performance is compared to that of NMPC that uses a direct simultaneous optimization method. The results show that the proposed algorithm (i) can enforce feasible operation for different uncertainty realizations both within batch or from batch to batch, and (ii) is significantly faster than direct simultaneous NMPC, especially at the beginning of the batch. In addition, a modification of the PMP-based NMPC scheme is proposed to enforce active constraints via tracking.

1. Introduction

Batch and semi-batch processes have wide application in the specialty industries for the production of low-volume, high-added-value products. Typical examples are pharmaceuticals, polymers and food. With increasing competition in industry and stricter environmental regulations, the optimal operation of batch processes plays an important role toward increased profitability. The inherently transient behavior as well as the presence of strong nonlinearities and of path and end-point constraints result in challenging optimization problems. Moreover, the lack of accurate models brings about considerable plant-model mismatch (Terwiesch et al., 1994; Bonvin, 1998; Srinivasan et al., 2003b; Jung et al., 2015). Hence, the open-loop implementation of off-line computed optimal control profiles may result in sub-optimal, or worse, infeasible operation. In addition, the operating conditions might change from batch to batch and cause unacceptable variations of product quality. Consequently, the application of measurement-based, optimizing feedback schemes is of great importance for semi-batch processes (Eaton and Rawlings, 1990; Ruppen et al., 1995; Ruppen et al., 1998; Bonvin et al., 2001; Bonvin et al., 2006; Kadam et al., 2007; Welz et al., 2008; Mesbah et al., 2011)

Model predictive controllers (MPC) have been used extensively in industry (García et al., 1989; Qin and Badgwell, 2003). On the basis of a (most often linear) process model, these controllers predict the future behavior of the states and outputs. At each iteration, the algorithm updates the initial conditions using measurements and solves a dynamic optimization problem for some cost function such as the minimization of a tracking stage cost or the maximization of a final cost. Only the first part of the computed optimal inputs is implemented, then the horizon is shifted by one sampling time and the procedure is repeated iteratively. Since MPC is

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http://dx.doi.org/10.1016/j.compchemeng.2017.08.010
0098-1354/

capable of addressing multivariable constrained nonlinear systems and can use different types of models and performance criteria, it possesses a suitable and flexible structure for real-time optimizing control (Diehl et al., 2002; Adetola and Guay, 2010; De Souza et al., 2010; Huang et al., 2010). A detailed discussion of and survey on MPC can be found in (Morari and Lee, 1999).

Because of the strong nonlinear behavior of batch processes, linear MPC is often not the method of choice for batch and semi-batch processes. Moreover, semi-batch processes usually require strictly constrained operation since the ability to influence the performance and feasibility of the process decreases with time (Bonvin, 1998). This motivates the use of shrinking-horizon nonlinear model predictive controllers (NMPC), for which the optimization is performed with respect to the full time horizon and includes both path and terminal constraints (Nagy and Braatz, 2003; Nagy et al., 2007).

Several studies on the applicability of NMPC to batch processes have been reported in the literature. Lakshmanan and Arkun (1999) used linear parameter-varying models for the estimation and control of nonlinear batch processes. Seki et al. (2001) proposed an NMPC structure for the industrial application on polymerization reactors. Nagy and Braatz (2003) studied a robust NMPC scheme for batch crystallization, whereby parametric uncertainties are taken into account explicitly. Valappil and Georgakis (2002) suggested a min-max NMPC scheme with successive linearization for the control of the end-point properties in batch reactors. Lucia et al. (2013) suggested a multi-stage NMPC scheme to deal with uncertainties, and a scenario-tree approach was used to optimize a semi-batch polymerization reactor. Recently, Jang et al. (2016) proposed a multi-stage NMPC scheme for semi-batch reactors using backoffs on path constraints. Binette and Srinivasan (2016) compared the performance of different tracking objectives for the NMPC of batch processes without parameters adaptation.

Nonlinear dynamic optimization (or optimal control) is at the core of NMPC and plays an important role in terms of implementation. The solution methods for dynamic optimization problems fall into the category of direct and indirect methods (Srinivasan et al., 2003b).

1.1. Direct methods

In direct sequential methods, the input vector is parameterized using polynomial functions, the states are integrated from their current values up to the final time, and the optimal input parameters are determined by a NLP solver (Vassiliadis et al., 1994; Srinivasan et al., 2003b). Since the states are not approximated, these methods are called 'feasible-path' methods. The computational complexity might turn out to be high, in particular for path-constrained problems, which is usually not acceptable for real-time algorithms.

In direct simultaneous methods (DSM), the optimal control problem is transformed to a NLP upon discretizing both the inputs and the states. Since the states are approximated instead of integrated, these approaches are called 'infeasible-path' methods. Direct simultaneous methods were reported to be effective for the optimization of large NMPC problems (Cervantes and Biegler, 1998; Biegler et al., 2002; Wächter and Biegler, 2006; Kameswaran and Biegler, 2006; Biegler, 2007; Huang et al., 2009; Jang et al., 2016). Zavala and Biegler (2009) introduced an 'advanced-step' DSM to deal with the feedback delay associated with the time required to compute the solution. Later, Huang et al. (2010) extended this method for the combination of NMPC and moving horizon estimation.

Another direct solution algorithm proposed for NMPC is the direct multiple shooting approach, which represents a mid-way between sequential and simultaneous algorithms. In this approach, the time interval is divided into stages, and the initial conditions of the stages are taken as decision variables for the optimization problem. This procedure is also an 'infeasible-path' method but the integration is as accurate as in sequential methods (Srinivasan et al., 2003b). Direct multiple shooting has been used extensively in NMPC problems (Keil, 1999; Bock et al., 2000; Diehl et al., 2002; Diehl et al., 2006; Schäfer et al., 2007; Findeisen et al., 2007). Mesbah et al. (2011) compared the performance of the DSM and direct multiple shooting algorithms for the real-time control of a fed-batch crystallizer.

1.2. Indirect methods

In indirect optimization methods, the optimization problem is reformulated as the minimization of an Hamiltonian function (Bryson, 1975). The reformulated problem is then solved to satisfy the necessary conditions of optimality (NCO) using Pontryagin's Minimum Principle (PMP). Indirect methods have been used to solve MPC problems in the literature. Cannon et al. (2008) designed a MPC strategy for input-constrained linear systems, whereby the inputs are represented in terms of co-states and the problem is solved using active-set methods. It was stated that the matrix factorizations performed by general direct solvers can be efficiently replaced by the computation of states and co-states using PMP. This way, the complexity per iteration increases only linearly with the length of the prediction horizon, which can be a computational advantage for batch processes that typically have large prediction horizons due to the shrinking-horizon approach. Kim and Rousseau (2012) used PMP for the optimal control of hybrid electric vehicles. Ali and Wardi (2015) proposed a multiple shooting method based on PMP, where the inputs can be expressed analytically in terms of states and co-states. Recently, Zhang et al. (2017) applied PMP in the context of MPC for a plug-in vehicle. In this method, the values of the co-states are determined by trial and error. For a more detailed review of the solution algorithms for NMPC, the reader is referred to (Cannon, 2004a,b).

However, until very recently (Aydin et al., 2017), there did not exist a fast convergent method to solve path-constrained optimal control problems using PMP (Hartl et al., 1995; Chachuat, 2007). Aydin et al. (2017) proposed an indirect, gradient-based dynamic optimization algorithm for the control of non-affine constrained semi-batch processes. The algorithm uses indirect adjoining to deal with path constraints, which allows the explicit calculation of inputs to meet the path constraints at each iteration step. The performance of PMP-based and DSM-based algorithms was compared on three different problems, with the indirect algorithm being found computationally superior, especially with finer discretization levels. In this work, we apply the convergent PMP-based algorithm proposed by Aydin et al. (2017) to the constrained NMPC problem of batch processes with both mixed and pure-state path constraints.

Furthermore, tracking the necessary conditions of optimality (NCO tracking) has also been proposed as a real-time optimization algorithm (Srinivasan and Bonvin, 2007). The optimal inputs are first computed via off-line optimization of the nominal model. The main assumption is that the solution structure (sequence and types of arcs) does not change with uncertainty. Hence, instead of performing explicit optimization at each NMPC iteration, the optimal solution structure computed off-line is tracked with the help of feedback controllers (Srinivasan and Bonvin, 2007; Srinivasan et al., 2008; Chachuat et al., 2009; Ebrahim et al., 2016).

The computational advantage of the PMP formulation represents the main motivation for this study. We propose to apply the novel PMP-based solution algorithm of Aydin et al. (2017) to the shrinking-horizon NMPC of *nonlinear* semi-batch processes in the presence of nonlinear pure-state and mixed-state path constraints. The effect of uncertainties is handled by the introduction of time-