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Nonlinear model predictive control of an industrial polymerization process



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ABSTRACT

Nonlinear model predictive control (NMPC) is used to maintain and control polymer quality at specified production rates because the polymer quality measures have strong interacting nonlinearities with different temperatures and feed rates. Polymer quality measures that are available from the laboratory infrequently are controlled in closed-loop using a NMPC to set the temperature profile of the reactors. NMPC results in better control of polymer quality measures at different production rates as compared to using the nonlinear process model with reaction kinetics to implement offline targets for reactor temperatures.

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1. Introduction

There are relatively few industrial applications of nonlinear model predictive control (NMPC) compared to linear model predictive control (LMPC) (Qin and Badgwell, 2003), and most of these are in the field of polymerization control. Industrial NMPC applications have been simplified to decrease the computational burden (Bindlish and Rawlings, 2003; BenAmor et al., 2004; Negrete et al., 2013) and results have been shown in simulation cases. A prototypical industrial polymerization control case study has been presented (Congalidis et al., 1989) and used to develop control strategies in simulations (Congalidis et al., 1989; Bindlish and Rawlings, 2003). A control scheme based on successive linearization has been used to track the optimal trajectory obtained by solving the unconstrained, nonlinear optimization problem offline without taking measured disturbances into account (Seki et al., 2001). Industrial implementation and results are reported for the controller, but the infrequent laboratory measurements are not used in the actual feedback control loop. Problems arise in applications of models to control actual industrial polymerization reactors due to significant process disturbances, modeling errors, and infrequent laboratory measurements. An important feature of industrial processes is that the key product quality measures are available only as laboratory measurements that have long sampling times

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http://dx.doi.org/10.1016/j.compchemeng.2014.11.001 0098-1354/© 2014 Elsevier Ltd. All rights reserved. with associated delays. A two-tier control scheme based on a linear model has been used to deal with the unavailability of on-line key product quality variable measurements (Ogunnaike, 1994). In the two-tier system, the set points for the on-line outputs are based on the targets for the laboratory outputs. Hence, the infrequent laboratory measurements are not used in the feedback control loop. Prior to the NMPC development for the industrial process discussed in this paper, a two-tier system that consisted of the non-linear process model with reaction kinetics was used to establish offline steady-state targets for reactor temperatures to maintain laboratory quality measures for polymer. There was no actual feedback control of laboratory quality measures (Fig. 1).

Dow's first application of a commercial nonlinear model predictive control technology that uses the laboratory quality measures in the feedback control loop is presented. The industrial nonlinear model predictive control problem has the following challenges

- Long laboratory sampling times for controlled polymer quality attributes (0.5–1 day)
- Varying dead times (2–7 days) and gains (multiplier of 1–20) for polymer quality attributes with respect to reactor temperatures
- Process models need to extend for extremely low feed rates (approximately 35% of normal rates)
- Process also occasionally operates with one of the seven reactors bypassed for maintenance
- For the first four reactors, recycle streams can only be manually set for heating or cooling



Fig. 1. Original control design for the process.

A linear model predictive controller (LMPC) will not be able to achieve the process objectives because there are strong nonlinear dependencies for polymer quality attributes with reactor temperatures and feed.

1.1. Process description and model

The physical details and chemistry for the industrial process are not disclosed because of proprietary reasons. The industrial polymerization process consists of seven well mixed reactors in series, where the extent of reaction is set by level and temperature in each reactor (Fig. 2). The copolymerization of monomer and comonomer is carried out using a catalyst to make a polymer characterized by polymer viscosity, unreacted monomer content and byproduct content. Comonomer composition in the feed is set at a stoichiometric excess value to minimize the unreacted monomer content in the polymer product. The catalyst dissolved in a solvent is also fed separately to the first reactor. The flow rate and composition of the feed streams are measured on-line along with the reactor temperatures and levels. Off-line laboratory measurements are made for the polymer viscosity, unreacted monomer content and byproduct content. Each reactor has a recycle stream, whose temperature is controlled by heating or cooling it. The reactor temperature is controlled by manipulating the recycle stream temperature.

2. Nonlinear model predictive control (NMPC)

2.1. Model development

A validated fundamental kinetic model based on first principles has been developed to capture the information in the process output measurements. Similar process models for a well-mixed polymerization reactor have been used for simulation of control strategies (Congalidis et al., 1989; Bindlish and Rawlings, 2003). The differential material balances including the rate expressions and the energy balance coupled with the equations for the physical phenomena constitute the dynamic process model. The following assumptions are made for developing the mass and energy balances in each reactor:

- Perfectly mixed tank
- · Linear mixing rule for reactor density

The fundamental model has been used historically to maintain polymer quality attributes by evaluating an off-line reactor temperature profile.

2.1.1. Bounded derivative network (BDN) model

Aspen Technology, Inc.'s Aspen Non-Linear Controller (Turner and Guiver, 2005; Naidoo et al., 2007) is used as the commercial NMPC controller, thereby requiring development of a boundedderivative-network (BDN) model instead of directly using the fundamental kinetic model. The bounded derivative network (BDN) model framework used by the commercial NMPC controller is the analytical integral of a neural network (Turner and Guiver, 2005) that offers the ability to specify minimum and maximum gains on each input-output relationship thereby circumventing the numerical problems associated with standard neural networks. Initial BDN model development was done by using simulation results of numerous fundamental kinetic model cases (approximately 50,000 cases) to cover the operating region of interest. These models were then deployed on-line, and tuned by comparison with real plant data. Over-parameterization of the BDN models was avoided to ensure extrapolation, and suitability for feedback control. The BDN model first derivatives of the controlled variables with respect to reactor temperatures and levels were examined over the operating range to ensure that they were monotonically increasing or decreasing, to match with those from the fundamental kinetic model. The nonlinear BDN model along with plant-model mismatch (*p*) can be discretized at the controller execution frequency (k) as

$$x_{k+1} = f(x_k, u_k, d_k)$$
(1)

$$y_k = h(x_k, u_k, d_k) + p_k \tag{2}$$

where *x* are the internal states of BDN, *u* are the manipulated inputs, *d* are the measured disturbances, *y* are the measured outputs, and *p* are the disturbances in output measurements. Plant-model mismatch is attributed to disturbances in output measurements instead of inputs or process in the NMPC formulation of Aspen Non-Linear Controller (Naidoo et al., 2007).

2.2. NMPC design

NMPC design in Aspen Non-Linear Controller (Naidoo et al., 2007) can be divided into following three parts

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