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Optimization-based strategies for the operation of low-density polyethylene tubular reactors: nonlinear model predictive control

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ABSTRACT

In this work, we present a general nonlinear model predictive control (NMPC) framework for low-density polyethylene (LDPE) tubular reactors. The framework is based on a first-principles dynamic model able to capture complex phenomena arising in these units. We first demonstrate the potential of using NMPC to simultaneously regulate and optimize the process economics in the presence of persistent disturbances such as fouling. We then couple the NMPC controller with a compatible moving horizon estimator (MHE) to provide output feedback. Finally, we discuss computational limitations arising in this framework and make use of recently proposed advanced-step MHE and NMPC strategies to provide nearly instantaneous feedback.

1. Motivation and background information

The decision-making hierarchy in many continuous chemical processes has been traditionally based on detailed *first-principles* steady-state models for economic optimization and empirical *data-driven* dynamic models for multivariable control (Marlin & Hrymak, 1996). Recently, it has been recognized that this model inconsistency can lead to infeasibility issues and performance deterioration (Engell, 2007; Yip & Marlin, 2004). In addition, the disturbances affecting the economics of many chemical processes occur at time scales that cannot be captured adequately by a steady-state optimization layer. The incorporation of first-principles dynamic models in the decision-making hierarchy opens the possibility to avoid these limitations and thus achieve unprecedented process efficiency. This can be done through economics-oriented nonlinear model predictive control (NMPC) or dynamic real-time optimization (D-RTO) schemes (Helbig, Abel, & Marquardt, 2000; Kadam et al., 2003). As expected, an important enabler of these control strategies is the development of efficient optimization strategies able to accommodate computational intensive dynamic models in on-line environments (Zavala, Laird, & Biegler, 2008).

In this work, we seek to integrate detailed first-principles dynamic models to optimize the operation of low-density polyethylene (LDPE) tubular reactor processes. LDPE is an important commodity polymer in today's economy due to its high flexibility and relatively low-cost (Knuuttila, Lehtinen, & Nummila-Pakarinen, 2004). LDPE is typically produced in tubular reactors by free-radical polymerization of ethylene at supercritical conditions (2000–3000 atm and 150–350 °C). A typical tubular reactor and corresponding temperature profiles for the reactor core and jackets are sketched in Fig. 1. LDPE reactors consist of long pipes (1–3 km) with small inner diameters (5–10 cm) and thick reactor walls (2–5 cm) which are divided into several reaction and cooling zones. These multi-zone configurations give rise to strong multivariable interactions along the reactor and thus lead to complex operating procedures. In addition, the operation is further complicated due to persistent dynamic disturbances such as fouling and initiator deactivation (Buchelli et al., 2005; Kiparissides et al., 2005; Luft et al., 1977). These disturbances have a strong impact on the process economics.

The potential economic benefits and high operational complexity of LDPE reactors have motivated research efforts in many areas. Extensive experimental studies have been performed in order to understand the principles governing these systems. This increased level of understanding has translated into numerous first-principles models of different fidelity and complexity (Goto et al., 1981; Kim

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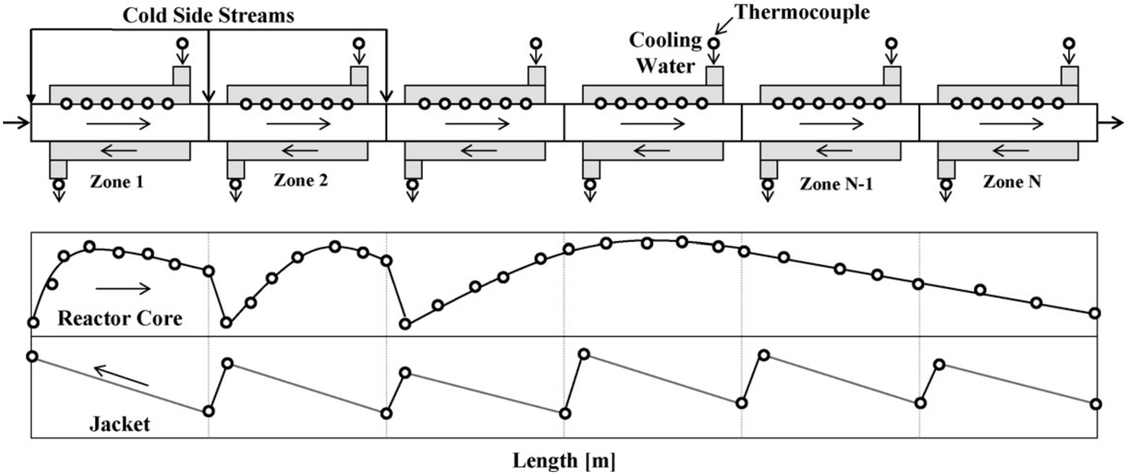

Fig. 1. Schematic representation of multi-zone LDPE tubular reactor (top). Typical reactor core and jacket temperature profiles (bottom).

& Iedema, 2004; Kiparissides, Verros, Pertsinidis, & Goosens, 1996; Kiparissides, Verros, & McGregor, 1993; Zabisky, Chan, Gloor, & Hamielec, 1992; Brandolin, Lacunza, Ugrin, & Capiati, 1996; Bokis, 2001; Häfele, Kienle, Boll, & Schmidt, 2006). The predictive capabilities of these models have also been evaluated and refined through systematic parameter estimation techniques (Kiparissides et al., 2005; Zavala & Biegler, 2006). Some of these models have been used for off-line tasks such as reactor design and dynamic transient analysis (Häfele et al., 2006; Pertsinidis, Papadopoulos, & Kiparissides, 1996). As a natural step, it is desired to use these models to perform on-line tasks such as economic optimization and model-based control. Zavala and Biegler (2008), demonstrated that significant economic benefits can be realized in LDPE reactors through model-based optimization strategies. In that study, a steady-state tubular reactor model described by large sets of differential and algebraic equations (DAEs) was used to evaluate the performance limitations of LDPE reactors in the presence of fouling disturbances. Zavala and Biegler (2008, 2009) demonstrated that detailed LDPE reactor dynamic models can be accommodated in on-line environments with the aid of current optimization capabilities to perform tasks such as moving horizon estimation (MHE) and nonlinear model predictive control (NMPC). These dynamic models are significantly more challenging since they involve computationally intensive partial differential, ordinary differential and algebraic equations (PDAEs) (Häfele et al., 2006). Here, we extend these results and derive a general NMPC framework to optimize the operation of LDPE reactors. We study the performance of both traditional NMPC designs in which the controller is used for regulation around a fixed target and we study the performance of economics-oriented designs in which the controller optimizes the process profitability and simultaneously performs regulation tasks. In addition, we discuss computational issues arising in the integration of NMPC and MHE tasks. Here, we will see that the on-line solution of the associated large-scale PDAE-constrained optimization problems gives rise to long feedback delays. Motivated by this, we make use of recently proposed synchronization or advanced-step strategies for NMPC and MHE based on nonlinear programming (NLP) sensitivity to overcome these limitations and provide nearly instantaneous feedback.

The paper is organized as follows: In the next section, we derive NMPC and MHE formulations for LDPE reactors. In Section 3 we present a short description of the computational strategies used to solve the associated PDAE-constrained optimization problems and to avoid long feedback delays. In Section 4 we discuss the performance of the NMPC framework under diverse scenarios and demonstrate the computational efficiency of the proposed strategies. The paper closes with Section 5 in which we present general conclusions and discuss directions of future work.

2. NMPC and MHE formulations

A typical operational hierarchy in industrial LDPE processes consists of a target-setting layer in which an operator receives the production schedule of different polymer grades. The operator sets the temperature profile of the reactor that is known by experience to give the desired polymer properties (e.g. melt index, density). The temperature targets are communicated to multiple PID controllers distributed along the reactor that try to keep the temperature profile at the desired target. The main tasks of the regulatory (PID) control layer are to reject short-term disturbances and to follow the temperature profile targets provided by the operator during grade changes.

As shown in Fig. 2, the PID controllers are normally grouped by zones in order to regulate the *local* temperature profile at each zone. Input variables such as the initiator flow, the jacket inlet temperature, the jacket inlet flow, and the side stream temperatures can be manipulated independently by each local set of controllers. The fouling onset is, in particular, a difficult disturbance to reject. As the reactor fouls, the controllers need to keep the local temperature profile at target. Because of this, they will tend to compensate by dropping the initiator flows and, implicitly, the production levels. It is important to emphasize that the controllers do not have any knowledge of the production levels of the reactor. Their objective is to keep the temperature profile at target which is set by the operator. Another problem that arises with a regulatory control architecture is that the controllers cannot foresee downstream (cascaded) interactions arising along the reactor. Because of this, the control of polymer properties at the reactor outlet can become cumbersome. It is believed that a *centralized* NMPC strategy able to

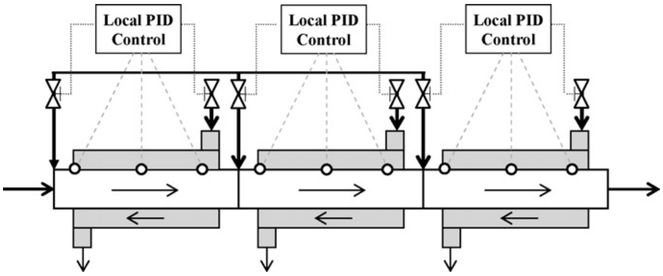

Fig. 2. Regulatory control structure of LDPE tubular reactors.