Integrated Dynamic Optimization and Scheduling of Polymerization Processes with First Principle Models

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Dedicated to Prof. Dr.-Ing. Günter Wozny on the occasion of his 70th birthday

An integrated dynamic optimization strategy is presented for block copolymerization processes. First the reactor model, which has unstable modes and may lead to unbounded profiles under certain design and operating conditions, is derived. Second, optimal recipes for operating of the copolymerization process are determined. Finally, an optimization strategy for the integration of scheduling and dynamic process operation for general continuous/batch processes is considered. The resulting approach leads to significant improvements in productivity, while maintaining safe operation and satisfaction of product specifications.

Keywords: Optimization, Polymerization, Scheduling

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1 Introduction

Optimization of dynamic systems was significant, high impact applications ranging from aeronautical applications [1, 2], robotics [3, 4], and process control [5]. In the design, operation and integration of chemical process systems, optimization of differential-algebraic equation models delivers efficient and safe operation in both batch and continuous processes. For the latter case, optimal transitions are needed to handle the dynamics of product grade changes, cyclic operations, catalyst deactivation over time, and fouling of heat transfer surfaces in a production cycle. For batch processes, optimal operating recipes need to be generated for dynamic operation of batch units. These batch units also need to integrate to the overall plant and to an operating cycle. This integration includes planning, scheduling, and control tasks that occur over broad time and length scales. For the integrated process to attain its peak performance, the optimization model and solution strategy must include an accurate behavioral description, which is best captured by a detailed, first principles process model. This study reviews an integrated dynamic optimization strategy for a ring-opening polymerization process for copolymer production. Through the application of advanced optimization strategies a significant performance improvement over conventional operations is demonstrated.

In the next section the statement of the dynamic optimization problem is introduced and a number of approaches to solve this problem, with a focus on the simultaneous collocation approach and a summary of its characteristics and advantages, are reviewed. The next three sections demonstrate the power of the simultaneous approach on the semi-batch ring-opening copolymerization process. Sect. 3 focuses on detailed reactor modeling through a population balance approach as well as a smaller model based on the method of moments. Sect. 4 describes and solves the dynamic optimization problem for the optimal recipe. Included in the problem formulation are the detailed kinetics, product specifications, and safety constraints. Also, both population and moment models are considered in the problem formulation and optimization of both reactor models are compared. Sect. 5 then considers the integration of batch processes with the logistics of scheduling and interactions with other units. An optimization formulation is briefly described that links the generation of optimal operating recipes together with a resource task network (RTN) for the production of multiple products in an overall plant. Finally, conclusions and directions for future work are given in the last section.

2 Dynamic Problem Statement

The optimization problem stated in the following form is considered:

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$$\min_{x(t),y(t),u(t),p} \Phi(z(t_f)) \quad \text{s.t.} \quad \frac{dz}{dt} = f(z(t), y(t), u(t), p), z(0) = z_0(p)$$
$$g_E(z(t), y(t), u(t), p) = 0 \qquad (1)$$
$$g_I(z(t), y(t), u(t), p) \leq 0$$
$$h_E(z(t_f)) = 0, \ h_I(z(t_f)) \leq 0$$

The variables in this optimization problem are the time-independent parameters p as well as differential state variables $z(t)$, algebraic variables $y(t)$, and control variables $u(t)$, which are functions of the scalar $t \in [t_0, t_f]$. As constraints differential and algebraic equations (DAEs) are given by Eq. (1) and without loss of generality it is assumed that this DAE system is index one.

As shown in Fig. 1, a number of approaches can be taken to solve Eq. (1). DAE optimization problems are solved using a variational approach or by various strategies that apply nonlinear programming (NLP) solvers to the DAE model. Until the 1970s, these problems were solved using an indirect or variational approach, based on the necessary conditions for optimality obtained from Pontryagin's Maximum Principle [1, 6]. For problems without inequality constraints, these conditions can be written as a set of DAEs. Obtaining a solution to these equations requires careful attention to the boundary conditions. Often the state variables have specified initial conditions and the adjoint variables have final conditions; the resulting two-point boundary value problem (TPBVP) can be addressed with different approaches, including single shooting, invariant embedding, multiple shooting, or through discretization methods such as collocation on finite elements or finite differences. On the other hand, if the problem requires the handling of active inequality constraints, finding the correct switching structure as well as suitable initial guesses for state and adjoint variables is often difficult. Early approaches to deal with these problems can be found in [1].

Methods that apply NLP solvers can be separated into two groups, sequential and simultaneous strategies. In the sequential methods, also known as control vector parameterization, only the control variables are discretized. In this formulation the control variables are represented as piecewise polynomials [7–9] and optimization is performed with respect to the polynomial coefficients. Given initial conditions and a set of control parameters, the DAE model is embedded within an inner loop controlled by an NLP solver. Parameters p that represent the control variables are updated by the NLP solver itself. Gradients of the objective and constraint functions with respect to input decisions are calculated either by direct sensitivity equations derived from the DAE system, or by integration of the adjoint equations; several codes were developed for both sensitivity approaches.

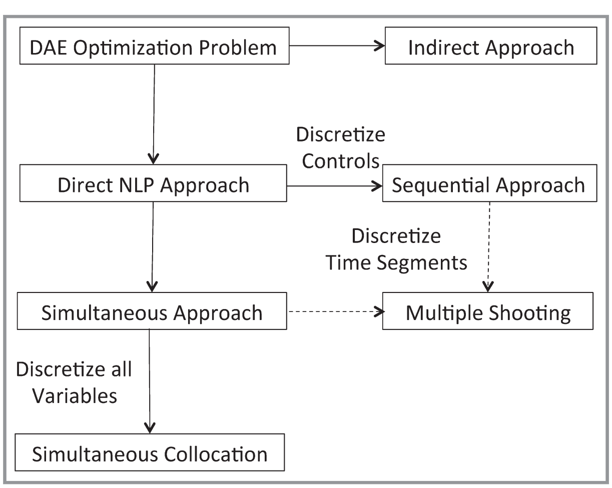

Figure 1. Solution strategies for dynamic optimization.

Sequential strategies are relatively easy to construct and apply, as they incorporate the components of reliable DAE and NLP solvers. On the other hand, repeated numerical integration of the DAE model is required, which may become time consuming for large scale problems. However, optimal control problems with many degrees of freedom require expensive (direct) sensitivity calculations that dominate the computation cost and also retain calculation noise that impedes the performance of the NLP solver. Moreover, sequential approaches are known to fail on unstable dynamic systems [10, 11]. Finally, state constraints can be handled only approximately by sequential methods, within the limits of the control parameterization.

Multiple shooting is a simultaneous approach that inherits many of the advantages of sequential approaches. Here the time domain is partitioned into smaller time elements and the DAE models are integrated separately in each element, along with corresponding sensitivity equations [12–14]. Control variables are parametrized as in the sequential approach and gradient information is obtained for both the control variables and the initial conditions of the state variables in each element. Finally, equality constraints are added to the NLP to link the elements and ensure that the states are continuous across each element. As with the sequential approach, inequality constraints for states and controls can be imposed directly at the grid points, and care is needed to avoid noisy and expensive sensitivity calculations. Finally, in the simultaneous collocation approach, both the state and control profiles in time using collocation of finite elements are discretized. This approach corresponds to a particular implicit Runge-Kutta method with high order accuracy and superior stability properties. Also known as fully implicit Gauss forms, these methods can be expensive (and are not widely applied) as initial value solvers. However, for boundary value problems and optimal control problems, this approach is essential as it requires far fewer time steps to obtain accurate solutions.