DATA-DRIVEN MODEL BASED CONTROL OF A MULTI-PRODUCT SEMI-BATCH POLYMERIZATION REACTOR†

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Abstract: Generic model control (GMC) has been successfully used for achieving tight control of batch/semi-batch processes. As the requirement to developing a mechanistic model can prove to be a bottle-neck while implementing GMC, many researchers have recently proposed GMC formulations based on black box models developed using artificial neural networks (ANN). The applicability of most of these formulations is limited to continuously operated systems with relative degree one. In addition, these formulations cannot handle constraints on inputs systematically. In the present study, ANN based GMC (ANNGMC) approach is extended to semi-batch processes with relative order higher than one. The nonlinear time-varying behaviour of batch/semi-batch processes is approximated using ANN model developed in the desired operating region. The ANN model is further used to formulate a nonlinear controller using GMC framework for solving trajectory-tracking problems associated with semi-batch reactors. The control problem at each sampling instant is formulated as a constrained optimization problem whereby the constraints on manipulated inputs can be handled systematically. The proposed controller formulation is used for solving trajectory-tracking problems associated with semi-batch reactors. The performance of the proposed control algorithm is evaluated by simulating the challenge problem proposed by Chylla and Haase (1993), which involves temperature control of a multi-product semi-batch polymerization reactor under widely varying operating conditions. The simulation exercise reveals that the performance of proposed ANNGMC formulation is comparable to the performance of the GMC formulation based on the exact mechanistic model, and is much better than PID controller performance.

Keywords: data-driven models; generic model control; artificial neural networks; semi-batch reactors; trajectory tracking.

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INTRODUCTION

The chemical industry has re-oriented from large-volume low-value production in continuous processes towards high-value low-volume production in batch processes due to the demand for a large number of specialty chemicals. Controlling a batch/semi-batch reactor along the optimal set point trajectory is one of the key problems in this area. Optimal operation of batch/semi-batch reactors involves two main tasks—generation of optimal set point trajectories, and controller design and synthesis for tracking of set point trajectories. Both these tasks have been handled predominantly with the help of first principles models, as reported in literature. Recently, Srinivasan *et al.* (2003) have reviewed and classified the methods for dynamic optimization of batch processes based on first principles models. The approaches available in the literature for trajectory tracking control of batch/semi-batch reactors can be classified as feed forward control, self-tuning and adaptive control, model predictive control, feedback linearization based control, estimation based control, coordinated control, and other control approaches (Berber, 1996). Prominent among these are global linearizing control, GLC (Kravaris and Chung, 1987), input–output linearizing control, IOLC (Palanki and Kravaris, 1997; Henson and Seborg, 1997) and generic model control, GMC (Lee and Sullivan, 1988).

GMC has been successfully used for achieving tight control of batch/semi-batch processes (Lee and Sullivan, 1988) and has therefore been considered for the present

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study. The relative degree of an output variable with respect to a manipulated input variable can be viewed as the smallest order of the output derivative that is directly influenced by the manipulated input. The basic GMC of Lee and Sullivan (1988) and some later versions of GMC (Dunia and Edgar, 1996; Xie *et al.*, 1999; Guo *et al.*, 2001) are limited to relative degree one systems and cannot be directly applied for higher relative degree systems, which are quite common in chemical engineering systems. The most commonly controlled variable in continuous or batch reactors is the reactor temperature and the jacket fluid flow rate is generally employed as the manipulated input variable. If the jacket fluid dynamics is negligible, this system becomes a relative degree one system. However, in a practical scenario, jacket fluid dynamics may not be negligible, and in such cases, the relative degree of the system for the same controlled output—manipulated input combination becomes two since the second order time-derivative of the reactor temperature is explicitly dependent on the jacket fluid flow rate. Even in the case where jacket fluid dynamics are not considered, if the concentration of one of the components is considered as the output variable to be controlled using coolant flow rate as the manipulated input (Ge *et al.*, 1999) or using temperature of the feed stream as the manipulated input (McLain *et al.*, 1996), the input–output combination becomes a relative degree 2 system. Another example of relative degree two system is the number average molecular weight control in a polymerization reactor using inlet initiator flow rate as the manipulated input (Sangeetha *et al.*, 1999). Henson and Seborg (1997) discuss the difficulties encountered in controlling higher relative degree systems, especially in the presence of load disturbances that exhibit an equal or lower relative degree with respect to the same output variable. Some versions of GMC have been proposed for higher relative degree systems (Rani and Gangiah, 1996; Wang *et al.*, 2003, 2004) based on the dynamic or steady state model based on first principles.

The most difficult and time-consuming step in implementation of different schemes of GMC is the development of a reliable first principles model for the process under consideration. Also, most of these schemes are developed under the assumption that all the state variables are either measured or can be accurately estimated from the available measurements, which may not be a realistic assumption in many practical situations. Data-driven black-box models, on the other hand, have gained significance as alternatives to first principles models. Rani and Gangiah (1991) have proposed an adaptive generic model control (AGMC) approach with the help of a model based on measured input output data, which does not require exact knowledge of the underlying physical processes. The parameters of the model are estimated at every sampling instant by recursive least squares (RLS) method.

During the last decade, ANNs have gained importance as versatile data driven structures for modeling nonlinear steady state as well as dynamic processes (Bhat and McAvoy, 1990). The ability of neural networks to learn complex nonlinear relationship has been exploited for the development of black box models. The most commonly employed neural networks have been the sigmoidal activation function based feed forward neural networks. Most of the ANN models have been NARX (nonlinear autoregressive exogenous) or NOE (nonlinear output error) type nonlinear difference equation models relating the input and output measurements (Su and McAvoy, 1997). Baughman and Liu (1995) have described the theory and applications of ANNs in different areas including data analysis, fault diagnosis, process modelling, identification and control. Hussain (1999) has reviewed the applications of neural networks in chemical process control by classifying them into model predictive control, inverse model based control and adaptive control methods, illustrating the tremendous prospects of neural networks in process control.

Recently, Rani and Patwardhan (2004) have proposed a novel data-driven approach for modelling and optimal set point generation for a batch/semi-batch process with the help of ANNs. There have also been some attempts to use ANNs for trajectory tracking in batch reactors. Chen and Huang (2004) have employed ANNs to model the batch reactor and used its linearized version at every sampling instant to update the tuning parameters of a PID controller. Horn (2001) has proposed a method to derive control law using input–output linearization approach with the help of ANN models, and illustrated its applicability through control of a batch polymerization reactor.

GMC formulation based on artificial neural networks (ANN) has been proposed for control of continuous processes. Ramchandran and Rhinehart (1995) and Dutta and Rhinehart (1999) have used ANN to model inverse of steady state map of a nonlinear process and further used it in GMC framework to derive a multivariable controller. This approach cannot be extended to batch/fed-batch operation as steady-state map cannot be defined for a batch process. Henson and Seborg (1997) and Piovoso *et al.* (1992) have reported an ANN based GMC approach for temperature control in a CSTR system using the cooling jacket temperature as the manipulated variable. By this approach, a grey-box model is developed whereby a part of the control affine model developed using material and energy balances is constructed using ANN. While development of such grey-box model is an interesting concept, it cannot be generalized to deal with systems with arbitrary form of nonlinearity and higher relative degree. As a consequence, the applicability of ANN based GMC approaches discussed above has been limited to continuously operated processes with relative degree one. Moreover, no attempt has been made so far to apply ANN based GMC approaches to batch/semi-batch processes.

While formulating any advanced control scheme, apart from the need to develop an accurate description of the process dynamics, an important consideration is ability of the control scheme to deal with operating constraints. The initial focus of research in GMC literature has been on deriving unconstrained closed form control laws. However, later there have been some attempts to incorporate constraints handling ability in the mechanistic model based GMC formulations. Brown *et al.* (1990) have incorporated general nonlinear constraints and solved a nonlinear optimization problem at each sampling instant. Further, Zhou *et al.* (1990) proposed an adaptive approach within GMC to accommodate the constraints by adapting one of the two GMC parameters, which is solved iteratively at each sampling instant. For higher relative degree systems, Rani and Gangiah (1996) have proposed a constrained non-iterative version of GMC with the help of a predictive formulation. Among the various ANN based GMC formulations, Dutta and Rhinehart (1999) have proposed a formulation that can systematically accommodate constraints on manipulated inputs. This approach, however, is based on ANN