

Open/Closed Loop Bifurcation Analysis and Dynamic Simulation for Identification and Model Based Control of Polymerization Reactors

M.P.Vega^{a*} and M.R.C. Fortunato^a

^a Universidade Federal Rural do Rio de Janeiro – Departamento de Engenharia Química
BR-465, km 7, Seropédica, Rio de Janeiro, Brasil, CEP. 23.890-000

Abstract

All steps of nonlinear system identification represent very challenging theoretical and practical problems, for a general theory is not available. As a result, further investigation on systematic techniques for nonlinear model validation is a relevant research issue that needs to be explored for proper model based controller implementation. Bifurcation analysis and dynamic simulation were employed for proper model identification and synthesis of model based controllers. The nonlinear model based control of batch and CSTR polymerization reactors are analyzed, as a case study. It is suggested that dynamic simulation analysis and the investigation of bifurcation diagrams (open/closed loop analysis), using reactor jacket temperature and weight average molecular weight set point as the bifurcation parameters, should be included as a synthesis criteria for nonlinear identification and model based control purposes.

Keywords: Model based control, Stability analysis, Polymerization, Dynamics

1. Introduction

As pointed out by Pearson and Ogunnaike (1997), a well-developed theory for nonlinear system identification is not available. Vega *et al.* (2001a, 2004) developed investigations on systematic techniques for nonlinear model validation using bifurcation diagrams.

Advanced controller design techniques take nonlinear behavior of the process into account. This category of methods includes feedback linearization and nonlinear model predictive control. In the case of model based process control, simplicity is a very important required characteristic, as the model has to be solved many times at each sampling interval. One typical example is the nonlinear model predictive control (NMPC), where an optimization problem based on the internal model has to be solved iteratively at each sampling interval (Henson, 1998).

Bifurcation analysis and control theory are two areas of research that have been developed independently from one another. Bifurcation analysis by continuation involves linearizations of generally nonlinear process models. This often causes confusion as readers assume that linearizations inevitably imply that the analysis is local

* Author/s to whom correspondence should be addressed: vega@ufrj.br

only. Bifurcation analysis by continuation can in fact be used for more than local analysis of nonlinear systems, despite using linearizations, for they are carried out along curves of steady states (Hahn *et al.*, 2004).

While both bifurcation analysis and nonlinear control theory deal with stability of nonlinear dynamic systems, the vast majority of the literature on bifurcation analysis has nevertheless focused on open-loop processes. Exceptions include Zhang *et al.* (2002) that performed bifurcation analysis on the open loop process in order to determine appropriate operating points for designing a controller. Chen *et al.* (2000), Recke *et al.* (2000) and Mönnigmann and Marquardt (2002) studied bifurcation control field: control of the dynamic behavior in the parametric vicinity of a bifurcation. Stability analysis was performed at one operating point (Ananthkrishnan *et al.*, 2003; Chang and Chen, 1984), for varying a parameter of a model (Paladino and Ratto, 2000) or the gain of a PI controller (Giona and Paladino, 1994) or the gain of a P controller (Cibrario and Lévine, 1991). Hahn *et al.* (2004) implemented bifurcation analysis to a closed loop system using state feedback linearization controller.

The main objective of this paper is using open/closed loop bifurcation analysis for proper nonlinear empirical model (internal model) and model based control (nonlinear model predictive control) synthesis. The solution polymerization in CSTR and batch reactors is studied. The methodology for confident identification and model-based control uses open/closed loop bifurcation and dynamic simulation analysis. As a result, the methodology should be included as genesis criterion in the nonlinear system identification/control scenarios.

2. Bifurcation analysis and dynamic simulations

Bifurcation theory provides tools for a system stability analysis under its parametric changes. As the parameters undergo changes, the existence of multiple steady states, sustained oscillations and traveling waves might occur for highly nonlinear processes (Ray and Villa, 2000).

The quality of the different models was evaluated by comparing their dynamic structure (attractors and respective stability characteristics) to the dynamic behavior of the “real” plant for the CSTR configuration. In order to do that, bifurcation and stability analyses were carried out to unveil attractors, employing well-known continuation methods. The computations presented in this paper were carried out with routines provided by AUTO (Doedel, 1986). Branches of steady state solutions and periodic solutions were calculated with the arc-length method developed by Keller (1977). Nonlinear system theory states that if all eigenvalues of the Jacobian matrix lie in the open left half of the complex plane, the system is stable. Conversely, the steady state is unstable if the Jacobian matrix has at least one eigenvalue in the open right half of the complex plane. The empirical model (internal model based on neural networks) is described as a discrete model, so that the stability characteristics are determined by the eigenvalues of the Jacobian matrix of the nonlinear map, which relates present data with the future process output. The stability characteristics of the closed loop (discrete system) are also determined by the eigenvalues of the Jacobian matrix of the nonlinear map: Steady states are stable if all eigenvalues of the Jacobian matrix are inside the unity circle. If any of the eigenvalues is outside the unity circle, the solution is unstable. At a Limit

Point, an eigenvalue becomes identically equal to +1. At this point, multiple steady state solutions usually appear and a change in stability occurs. At a Hopf (Thorus) Bifurcation Point, a pair of complex eigenvalues crosses the unit circle with non-zero imaginary component and a branch of oscillatory solutions may appear. At a Period Doubling Bifurcation Point an eigenvalue becomes equal to -1 and branches of periodic solutions usually develop. AUTO automatically detects bifurcation points and provides routines for computation of the multiple steady state solutions, oscillatory and periodic solutions that arise at these special points. Unstable behavior usually occurs in the vicinities of these bifurcation points.

The quality of the different models describing a batch polymerization reactor was evaluated by analyzing their dynamic structures. It is assumed here that a good empirical model should exhibit a dynamic behavior that resembles the one of the original process. This means that the empirical models should present the same modes of operation of the original process. Therefore, in our particular case, a good empirical model should not display multiple solutions and unstable operation conditions.

As a result, the identification of the bifurcation diagram and dynamic structure of open/closed loops may allow the understanding of how and why the empirical models fail at certain process operation conditions, even when allowing a satisfactory one step ahead prediction of process dynamics, required by traditional validation methods (Srinivas *et al.*, 1995), producing spurious controller performances.

3. The process analyzed

The solution styrene polymerization was the system employed for illustrating the methodology that develops reliable model identification and model based control of weight average molecular weight. Detailed description of the process may be found elsewhere, Vega *et al.* (2001a). There is much interest in the in-line monitoring and control of molecular weight distributions, as this may be regarded to be among the most important molecular properties of polymer resins. However, the analysis of polymer chain length using GPC, SEC, and light scattering, requires very expensive, sophisticated, time-consuming and unreliable (at industrial environments) instruments. From a practical point of view, the whole molecular weight distribution is not needed and significant amount of information about the end-use properties may be provided by the leading moments of the molecular weight distributions, such as the weight average molecular weight. Vega *et al.* (2001b) developed a simple viscometrical method for in-line monitoring and control of weight average molecular weight in solution polymerizations. As a result, the weight average molecular weight is the polymeric property chosen for being controlled.

The dynamic simulation of the batch polymerization model is shown in Figure 1. The CSTR bifurcation and stability analysis diagrams are rendered in Figures 2 and 3. The CSTR model presents a stable steady state solution branch.

4. Results and discussion

Nonlinear system identification involves model parameters selection, determination of the forcing function, which is introduced into the plant to generate the output response,

estimation of model parameters and comparison of plant information and model predictions for data not used in model development. All steps represent very challenging theoretical and practical problems, for a general theory is not available. The neural network (NN) approach has proved to be a useful tool and is the most popular framework for empirical model development.

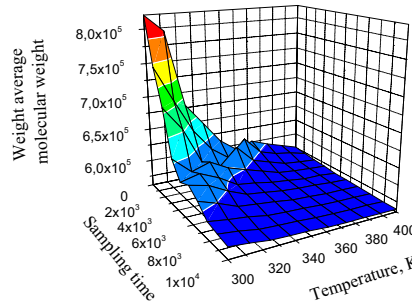


Figure 1. The batch model dynamic simulation

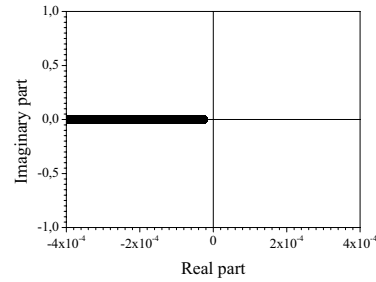
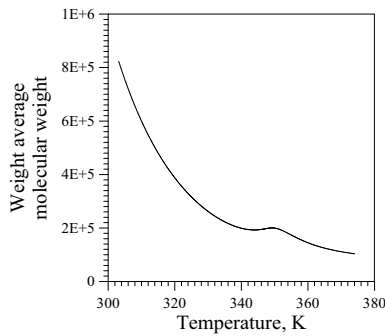


Figure 2. The CSTR model bifurcation diagram Figure 3. The CSTR model stability analysis

In order to control polymer quality (weight average molecular weight) a NMPC strategy was developed (Henson, 1998), using a NN as the internal model, named empirical model, by manipulating the reactor jacket temperature. All NNs present 2x4x1 architecture (reactor jacket temperature and conversion as inputs and weight average molecular weight as output).

Empirical models were compared with the corresponding bifurcation diagrams and dynamic simulations of the phenomenological models, regarded as the real processes. Vega *et al.* (2004) pointed out that the use of traditional validation tests was not enough to guarantee successful use of NNs as the internal models of NMPCs. Care must be taken regarding the strategy for data generation, as the simple manipulation of the number of data points, neuron activation functions, NN architecture and initial guesses used for NN training are not enough to guarantee the building of proper models. As shown in Figures 4 and 5, the complex dynamic behavior displayed by the model (build with incomplete data set) may be completely different from the one displayed by the plant, resulting in poor control efficiency. Good controller performance was obtained when model and plant showed similar dynamic simulations.

The empirical model bifurcation diagram (Figure 6) displays a CSTR phenomenological model similar behavior. All Floquet multipliers are inside the unity circle ensuring stable steady states (Figure 7). For closed loop bifurcation diagram synthesis (Figure 8) the output of the controller (reactor jacket temperature) serves as input to the system and has to be removed from the set of variables to be used for bifurcation analysis. Then, the set point of the system (weight average molecular weight) is the continuation parameter. As a result, the analysis can be performed over an entire operation region of the process rather than for a particular fixed value of the set point. Figure 9 shows that the closed loop system remains stable under parametric uncertainty and unmodeled dynamics over the entire operating region. Requiring stability of the closed loop system over the entire operating region is important because bifurcation analysis only results in steady state information, and it has to be ensured that the system trajectories cannot leave the regions of attraction of the steady state operating point.

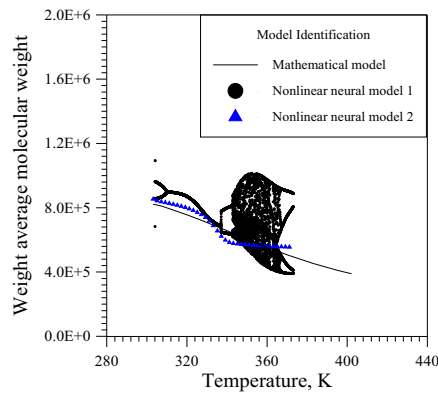


Figure 4. Model identification- batch model

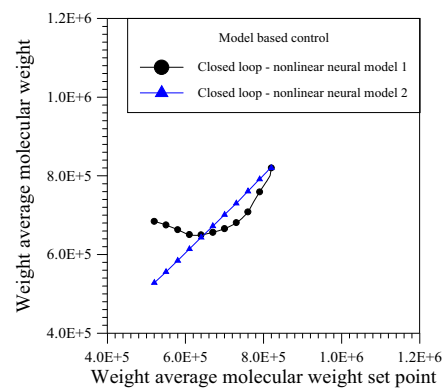


Figure 5. Model based control - batch model

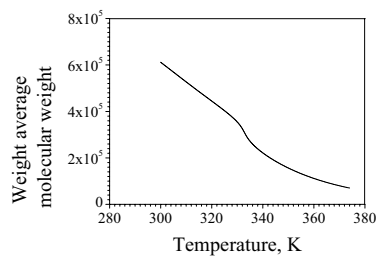


Figure 6. CSTR open loop bifurcation diagram

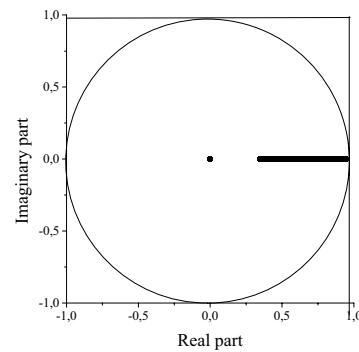


Figure 7. CSTR open loop stability analysis

5. Conclusions

It was observed that nonlinear models built to represent polymerization reactors may present incompatible complex dynamic open loop behavior, producing incompatible controller performance, unveiled by dynamic simulations and bifurcation theory. Bifurcation diagrams and dynamic behavior indicate whether spurious model responses

are present and, therefore, indicate whether additional effort is needed for proper model development. Bifurcation analysis was used as an efficient tool for validating nonlinear models, which were built in a supervisory fashion, using available first principles mathematical modeling data. Following the data selection procedure (number, range and distribution) for nonlinear system identification, unknown systems can be unveiled if the convergence of the bifurcation diagram to a final structure is used as a quality index in an iterative procedure. This sophisticated validation procedure is indicated for complex units operating in a large range of operating conditions and using nonlinear model based controllers. Finally, it was shown that bifurcation analysis was successfully implemented for closed loop system analysis under phenomenological model and plant (internal model) mismatch of a NMPC scheme.

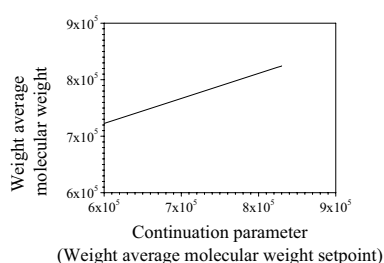


Figure 8. CSTR closed loop bifurcation diagram

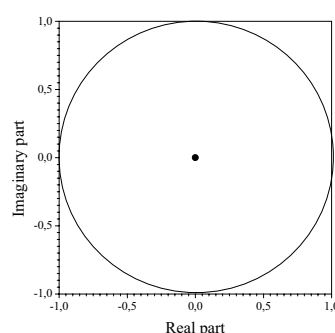


Figure 9. CSTR closed loop stability analysis

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