CONTROLLER VERIFICATION FOR POLYMERIZATION REACTORS

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Abstract

A methodology for verifying the stability and performance of a controller, when the process model is incompletely known, is demonstrated for a polymerization reactor. Model uncertainty arises when either the parameters are known only approximately (parametric uncertainty), or when the form of the equations is not known exactly (non-parametric uncertainty). Two techniques are used to solve the semi-quantitative models to predict all of the possible behaviors. One involves qualitative analysis, implemented in the NSIM program, that uses symbolic manipulation to build bounding equations, and the other is a non-parametric Monte-Carlo technique. Temporal logic operators are used to formalize the posing of and automatic answering of qualitative questions about the response of the system.

Keywords

Controller verification, Non-parametric uncertainty, Monte-Carlo simulations, Qualitative analysis, Styrene polymerization.

Introduction

Most chemical processes are modeled by ordinary differential equations (ODEs) that exhibit substantial uncertainties in the model parameters, inputs and initial conditions. Often, the terms and the form of the equations are uncertain because the mechanisms are not well understood. As an example, the dependence of the rates of reaction on temperature and composition is often not accurately known for complex reaction mechanisms. In these cases, experimental data can help to determine bounding envelopes, using the methods described by Kay and Ungar (1993). The true functions are not likely to be coincident with either of the envelopes, but confidence levels can be established that they lie between them. Although techniques exist to deal with parametric uncertainty, the representation and simulation of nonlinear models with inexact functional relationships has not been addressed as effectively.

Several qualitatively distinct behaviors may be consistent with a single such *semi-quantitative* model. For example, an increase in the reactor temperature may result in either a desirable increase in the reaction rates or undesirable instability, depending on the values of the parameters. Two techniques are introduced to solve semi-quantitative models to predict all of the possible behaviors. One involves qualitative analysis, implemented in the NSIM program, that uses symbolic manipulation to build bounding equations, and the other is a non-parametric Monte-Carlo technique. Then, *temporal logic* operators are used to formalize the posing of and automatic answering of questions of the type: "Can the system operate adequately if a disturbance/fault occurs?" This methodology applies for the automatic verification of control actions to guarantee that processes will not move into hazardous operating regimes when faults are encountered; that is, in the design of *safety net* control actions. With such off-line verification, large overdesign factors, that are often used to compensate for model uncertainties, can be avoided.

Simulation of Uncertain Models

In this section, the two techniques are described. It is assumed that the unknown functions, $y = f\{x\}$, are bounded between envelopes, such that $f_\ell\{x\} \leq y \leq f_u\{x\}$, and are

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monotonic (Fig. 1). The monotonicity assumption is very important for the analysis, but is not overly restrictive, since any non-monotonic function can be constructed by combining monotonic ones. In addition, it is often known that physical quantities are related to each other monotonically, even though the relations may not be known accurately; e.g., reaction rates increase monotonically with temperature, and friction factors increase monotonically with velocity.

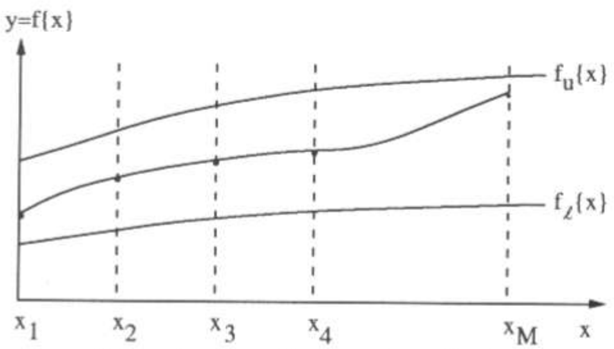

Figure 1. Bounding envelopes for f{x}.

The two techniques presented herein are based on entirely different philisophies. The first involves a "worst-case", deterministic analysis, that derives ODEs whose solution is guaranteed to bound all of the solutions of the inexact model, and is based on the NSIM algorithm. The second is a statistical analysis, that extends the Monte-Carlo technique for systems with non-parametric uncertainty. The advantages and disadvantages of each approach are discussed below.

The NSIM Algorithm

The QSIM algorithm (Kuipers, 1986) provides a framework for developing models in the form of qualitative differential equations (QDEs), which are abstractions of ordinary differential equations (ODEs), where the values of the variables are described qualitatively and the functional relationships between the variables may be known incompletely. The constraints are qualitative expressions involving the common mathematical operations, such as addition, multiplication, and differentiation as well as monotonicity. Given a QDE and a qualitative description of an initial state, QSIM derives a tree of qualitative state descriptions, where the paths from the root to the leaves of the tree represent the possible behaviors of the system.

In NSIM (Kuipers, 1989; Kay and Kuipers, 1993), an extension of QSIM, parameters may be assigned lower and upper bounds and monotonic functions may be bounded by lower and upper envelopes, thus forming Semi-Quantitative Differential Equations (SQDEs). These permit NSIM to eliminate behaviors that are inconsistent with the numerical information, while describing the remaining behaviors more quantitatively. NSIM produces bounds on the trajectories of the state variables that are guaranteed to include *all* of the behaviors consistent with the approximate model.

Given a SQDE and an initial condition, NSIM derives and numerically integrates an "extremal" system of ODEs, whose solution is guaranteed to bound all of the solutions of the SQDE. This is referred to as NSIM *simulation*. The extremal system is generated automatically, using symbolic manipulation, based on a set of rules (Kay and Kuipers, 1993). An extremal equation is a bound on the first derivative of a state variable. Minimal and a maximal equations are derived for the state variables, defining a *dynamic envelope* for each variable, and hence, an n-th order system is transformed to a 2n-th order system. As a result, the extremal ODEs are not generally members of the class of ODEs represented by the SQDE. Therefore, the dynamic envelopes do not necessarily have the same shape as the behaviors of the SQDE.

The extremal system is integrated using a standard Runge-Kutta technique. It is proven theoretically (Kay, 1991) that, when the extremal system bounds the solution of the SQDE at $t = 0$, it bounds the solution for all times.

A SQDE is an abstraction of an ODE with incompletely specified functions and parameter values. One NSIM "simulation" covers an infinite number of models. Since the NSIM bounds are guaranteed to bound all the solutions to the SQDE, NSIM can be used for automatic proof construction. However, the main disadvantage of this technique is that the bounds are conservative, as illustrated by Gazi et al. (1994).

The Non-parametric Monte-Carlo Technique

To extend the Monte-Carlo technique to handle non-parametric uncertainty, a large number of monotonic functions are randomly generated within the envelopes that bound the incompletely known monotonic functions. Each generated function is incorporated into the ODEs that model the process, which when integrated produce trajectories of the state variables that are systematically checked for "interesting" behaviors, as described in the next section. This is accomplished using the following algorithm:

1. M intervals in x are formed.
2. At $x = x_1$, y_1 is selected randomly such that $f_\ell\{x_1\} \le y_1 \le f_u\{x_1\}$.
   At $x = x_k$, y_k is selected randomly such that $f_\ell\{x_k\} \le y_k \le f_u\{x_k\}$ and $y_k \ge y_{k-1}$, $k = 2,\ldots,M$.
3. The points (x_k, y_k), $k = 1,\ldots, M$, are connected with straight lines.
4. The system of ODEs is integrated.
5. Steps (2)-(4) are repeated.

In this analysis, it is important to ensure a satisfactory coverage of the space of possible functions. Gazi et al. (1995) show that the monotonicity constraint clusters the generated functions close to the upper envelope, as x increases, when the y's are selected from uniform distributions. To avoid this, y_1 and y_M are selected randomly first, and then the x coordinate is subdivided recursively.

A large number of simulations (one with each generated function) is required, and the results are guaranteed to include all possible behaviors only in the limit as the number of samples approaches infinity.

Controller Verification

During process design, with substantial uncertainties present, the specific trajectories produced by numerical simulations may be unreliable. It should be helpful to the engineer, in carrying out process and controller design, to prepare qualitative descriptions of the possible closed-loop behaviors. With this, the engineer would establish the bounds on a desired *nominal region of operation* and automatically verify off-line whether, for example, the controller would return the process to a steady state, within the nominal region, in the face of anticipated disturbances and faults.

Given the nominal, semi-quantitative, model for the process and the controller, as well as the potential faults, the proposed verification scheme is as follows. The engineer asks a question of the type, "What may happen if this fault occurs?" In response, the fault model is automatically built and integrated (using either of the techniques described above). Then, *temporal logic operators* (Emerson, 1990) are used to express formally the user-supplied questions about the system behavior, and provide qualitative answers.

A similar scheme has been applied for the verification of discrete-event control systems by several authors. For example, Moon et al. (1992) build a tree that includes all of the possible behaviors of the system (a succession of discrete events in time) and check it systematically to determine the truth of the question. Herein, the trajectories of the state variables produced by each Monte-Carlo simulation may be viewed as one behavior.

Table 1. Temporal Logic Operators.

modal	temporal	logical
necessarily	always	and
possibly	eventually	or
	until	not

The temporal logic operators used are shown in Table 1. Through the modal operators, the user can specify whether the question must be true for all Monte-Carlo simulations (necessarily) or at least one (possibly). In the case of NSIM simulations, the modal operator is set to "necessarily" by default. For each individual trajectory, a question might refer to the whole time range (always), or only over time intervals (eventually, until). The logical operators are the conventional Boolean connectives. An example question expressed using the temporal logic operators is given in the next section.

Application to Styrene Polymerization

This methodology is illustrated for the free-radical polymerization of styrene in a jacketed CSTR (Figure 2; Higaldo and Brosilow, 1990). The objectives are to stabilize the reactor at an unstable steady-state and control the average molecular weight and the molecular weight distribution of the polymer. The flow rate of the cooling water, F_c, is used as the primary action for the control of the reactor temperature, with the monomer flow rate, F_m, the secondary control action in response to large disturbances. The flow rate of the initiator, F_i, is manipulated to keep the weight-average molecular weight, M_w, close to its setpoint. A combination of PID controllers, using sliding-gain scheduling, regulates the reactor in the face of uncertainties and large disturbances.

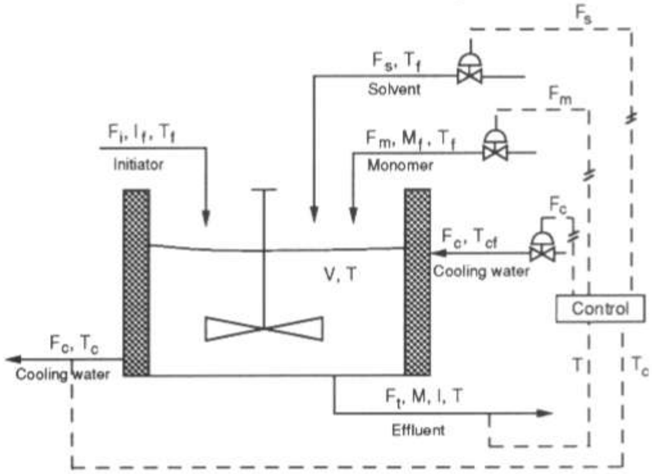

Figure 2. Schematic of a jacketed CSTR for styrene polymerization.

The models for the styrene polymerization reactor contain substantial uncertainties. As an example, the rate constant for the termination reaction is of the form, $k_t = k_{t0}\, g_t$, where k_{t0} is the value of the rate constant at very low monomer conversions, and is assumed to have an Arrhenius dependence with parametric uncertainty. g_t is a function that monotonically increases with temperature and decreases with reactor composition, reflecting the fact that k_t falls due to diffusion limitations at higher conversion. This functionality is unknown, but can be bounded by envelopes based upon experimental data (Fig. 3). Moreover, the weight-average molecular weight cannot be measured on-line. Rather, the viscosity is measured, but its relationship to M_w is uncertain.

Figures 4 and 5 show the response of the closed-loop system, as predicted by NSIM and Monte-Carlo simulations, respectively, in answer to the question:

"If the reactor temperature set-point increases by 6-8K, is it
(*necessarily* ((*always* (in nominal region)) *and*
eventually (steady-state))) ?"

where the "nominal region" of operation is defined such that, $340 \leq T \leq 360$ K, and $30{,}000 \leq M_w \leq 35{,}000$.

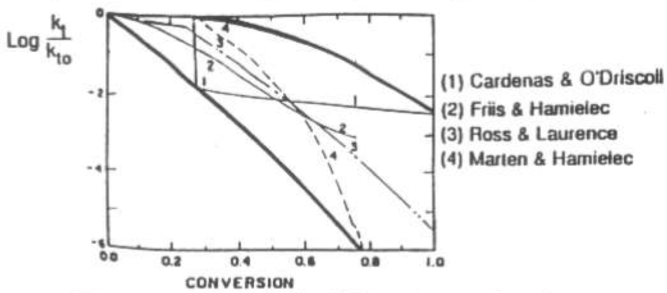

Figure 3. Bounds (bold lines) on g_t, based on experimental studies.

The NSIM bounds diverge, showing that unstable trajectories are possible, and hence, the answer "false" is returned. However, this is attributed to the conservatism of the NSIM bounds. On the contrary, the Monte-Carlo simulations predict tight bounds for all of the state variables, and hence, provide an affirmative response.

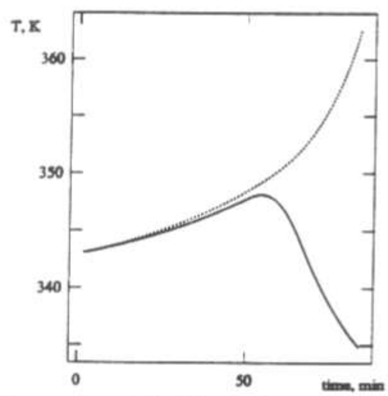

Figure 4. NSIM bounds on the reactor temperature, for a set-point increase by 6-8 K.

Conclusions

A methodology is introduced for the off-line verification of the stability and performance of controllers, when the process model has substantial, parametric and non-parametric, uncertainty. Two techniques are presented for the simulation of such semi-quantitative models. Although more expensive computationally than NSIM, with guarantees only in the limit of infinite samples, the Monte-Carlo method produces bounds that are not conservative, as illustrated for the design of a styrene polymerization reactor and its control system.

Acknowledgments

Partial funding provided by NSF Grant Nos. IRI-9216714 and DDM-9114080 is gratefully acknowledged.

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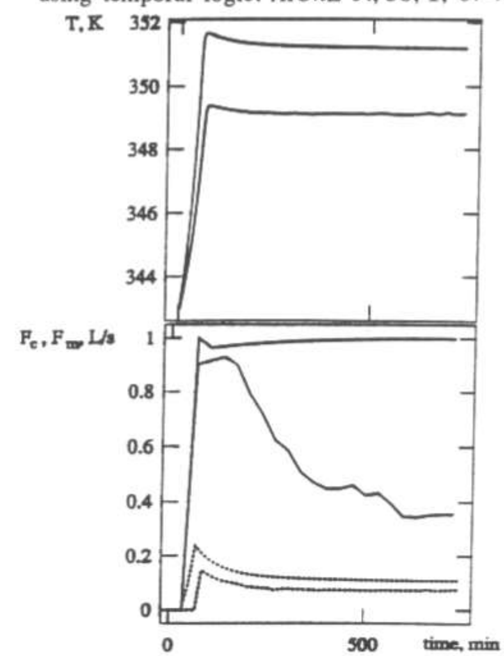

Figure 5. Monte-Carlo bounds on the reactor temperature, T, and the manipulated cooling water and monomer flow rates, F_c and F_m for a 6-8 K increase in the temperature set-point.