Guaranteed Steady-State Bounds for Uncertain Chemical Processes

Jan Hasenauer [*], **Philipp Rumschinski** [**], **Steffen Waldherr**[*], **Steffen Borchers**[**], **Frank Allgöwer**[*], and **Rolf Findeisen**[**]

[*] *Institute for Systems Theory and Automatic Control, Universität Stuttgart, Germany (e-mail: {hasenauer,waldherr,allgower}@ist.uni-stuttgart.de)*

[**] *Institute for Automation Engineering, Otto-von-Guericke-Universität Magdeburg, Germany (e-mail: {philipp.rumschinski, steffen.borchers,rolf.findeisen}@ovgu.de)*

Abstract: Analysis and safety considerations of chemical and biological processes frequently require an outer approximation of the set of all feasible steady-states. Nonlinearities, uncertain parameters, and discrete variables complicate the calculation of guaranteed outer bounds. In this paper, the problem of outer-approximating the region of feasible steady-states, for processes described by uncertain nonlinear differential algebraic equations including discrete variables and discrete changes in the dynamics, is adressed.
The calculation of the outer bounding sets is based on a relaxed version of the corresponding feasibility problem. It uses the Lagrange dual problem to obtain certificates for regions in state space not containing steady-states. These infeasibility certificates can be computed efficiently by solving a semidefinite program, rendering the calculation of the outer bounding set computationally feasible. The derived method guarantees globally valid outer bounds for the steady-states of nonlinear processes described by differential equations. It allows to consider discrete variables, as well as switching system dynamics.
The method is exemplified by the analysis of a simple chemical reactor showing parametric uncertainties and large variability due to the appearance of bifurcations characterising the ignition and extinction of a reaction.

Keywords: Steady-states, nonlinear dynamical systems, discrete variables, hybrid dynamics, semidefinite programming, CSTR

1. INTRODUCTION

In the chemical and biochemical processing industry one frequently has to face large modelling uncertainties and process disturbances. Precise reaction mechanisms and kinetic parameters might be unknown and operating conditions, e.g. feed flowrate, or feed temperature, can be time dependent. Additionally, many of the substances handled in a chemical plant are potentially dangerous, e.g. inflammable or explosive. Reactions can lead to the disposal of large amounts of thermal energy, what makes safety considerations necessary. Stationary temperature and pressure have to stay below critical values and for instance in pharmaceutical processes the variability within the drug production has to be restricted. Hence, a detailed analysis of the process uncertainty is essential.

In this paper we address the problem of determining the set of all feasible steady-states of a process, for a class of uncertain hybrid nonlinear differential algebraic systems. Using the set of feasible steady-states the stationary process uncertainty can be upper bounded. Furthermore, it can be used to check whether for all possible disturbances, parameter variations, and operating conditions the process operates within previously defined constraints. One exemplary question to be asked is whether thermal runaway of a chemical reactor can be avoided under specific failure situations.

The physical processes taking place in chemical plants mostly behave in a continuous fashion. There are, however important discrete phenomena like changes in the physical system, e.g. phase transitions, imposed qualitative changes caused by limitation of the equipment, e.g. limited tank capacity, discontinuous input signals and process faults (Engell et al., 2000). To capture continuous as well as discrete phenomena, regime based approaches are used to model the process behavior (Seborg et al., 1989; Murray-Smith and Johansen, 1997; Lennartson et al., 1996). Frequently, one refers to this kind of models as hybrid models, because they contain both discrete and continuous dynamical components and an interface describing the interaction of them.

For most nonlinear systems an analytical calculation of the set of steady-states is impossible. Therefore, during the last decade several methods have been developed for approximating the set of feasible states, in the context of reachability analysis. Those methods are rather efficient if the considered system is linear time-invariant (Girard

and Guernic, 1996) and also for uncertain linear systems some results exist (Girard, 2005). However, if the systems under consideration are nonlinear, the approximation of the feasible set is more difficult. Asarin and coworkers developed an approach for two-dimensional systems based on piecewise linear approximation (Asarin et al., 2003) and Ramdani et al. (2008) proposed a method for high dimensional uncertain nonlinear systems using guaranteed set integration, which yields good results for cooperative systems. Nevertheless, the performance of these methods strongly depends on the particular structure of the nonlinear system and in many cases the results are very conservative.

Due to this drawback of set-based approaches, for the analysis of nonlinear systems, often simple Monte-Carlo type methods are employed (Robert and Casella, 2004). However, such approaches only provide the complete set of possible steady states in the limit of infinite many samples, i.e. important solutions might be left out, especially for highly nonlinear systems.

The method derived in this paper follows the idea presented in the work of Waldherr et al. (2008). There, recent advances in the field of semidefinite programming (SDP) (Parrilo, 2000; Chesi et al., 2003) are employed to compute certificates that a given set in state space cannot contain a steady-state for any feasible model parameterization. A very similar approach was earlier proposed by Kuepfer et al. (2007) for parameter estimation and later extended to dynamical systems by Borchers et al. (2009). However, all these methods are restricted to systems described by polynomial vector fields, which is rarely the case for chemical processes. Furthermore, discrete variables or parameters, as might occur in the analysis of chemical and biological processes, have not been considered.

In the following, an approach will be presented, which overcomes this shortcoming and allows the outer approximation of the set of all feasible steady-states of a process described by uncertain hybrid nonlinear differential algebraic equations with non-polynomial vector fields. Thus, systems combining continuous dynamics with logic or discrete components can be studied. Furthermore, a more elaborate algorithm is proposed to obtain a more precise approximation of the set of feasible steady-states, in cases the considered system has multiple steady-states.

The remainder of this paper is structured as follows: In Section 2 the problem of bounding the set of steady-states for processes described by non-polynomial hybrid differential algebraic equations is presented. Section 3 formalizes the problem statement. In Section 4 the resulting feasibility problem is relaxed to a semidefinite program which is used by the algorithm outlined in Section 5 to estimate the set of feasible steady-states. In Section 6 we provide as an example the analysis of a CSTR, before final conclusions are provided

Mathematical notation: The space of real symmetric $n \times n$ matrices is denoted as $\mathcal{S}^n$. N_a^b denotes the discrete set $\{1, \ldots, n_a^b\}$, where n_a^b is the number of considered variables. The positive semidefiniteness of a quadratic matrix $X \in \mathcal{S}^n$ is denoted $X \succeq 0$ and the trace of X by tr X. The transposed vector $(x^d)^T$ is written as x^{dT}.

2. PROBLEM STATEMENT

The processes under consideration are supposed to be described by hybrid differential algebraic systems which exhibit both continuous and discrete dynamical behavior. Such a process description is quite general. It covers for instance reaction networks which allow phase transitions, as well as discrete variables/inputs such as the opening of a valve or the on/off status of a heater. Mathematically, we assume that the process is described by

$$0 = F^d(\dot{x}^d, x^d, p^d, u^d), \qquad x^d(0) = x_0^d \tag{1}$$

Here $x^d \in \mathbb{R}^{n_x^d}$ is the state vector, $p^d \in \mathbb{R}^{n_p^d}$ the vector of parameters, $u \in \mathbb{R}^{n_u^d}$ the vector of inputs (externally manipulated variables), and $F^d : \mathbb{R}^{n_x^d} \times \mathbb{R}^{n_x^d} \times \mathbb{R}^{n_p^d} \times \mathbb{R}^{n_u^d} \to \mathbb{R}^{n_x^d}$ the mapping for a given discrete decision variable $d \in \mathbb{N}$. The decision variable d is assumed to be time dependent with $d(t) \in \mathcal{D}$.

To derive such hybrid differential algebraic descriptions in which each node captures the dynamics under certain operating conditions and to define switching surfaces is often easier than deriving ordinary differential equation models, holding for all process configurations.

In the following we are interested in the steady-state behavior of (1). The problem under consideration is to find all possible, or at least an outer bound of all, steady states of (1):

Problem 1. (Set of feasible steady states): Given the sets $\mathcal{D} \subset \mathbb{N}$, $\mathcal{P}^d \subset \mathbb{R}^{n_p^d}$ and $\mathcal{U}^d \subset \mathbb{R}^{n_u^d}$, compute the set $\mathcal{X}_s^*$ which contains all feasible steady-states of (1).

Note that the set of feasible steady-states for a given decision variable $d \in \mathcal{D}$ is defined by

$$0 = F^d(0, x^d, p^d, u^d). \tag{2}$$

Hence problem 1 can be split into n_d subproblems, where n_d is the cardinality of $\mathcal{D}$. For each subproblem one obtains a set of feasible steady states

$$\begin{aligned}\mathcal{X}_s^{d,*} = \{x^d \in \mathbb{R}^{n_x^d} \mid \exists\, p^d \in \mathcal{P}^d, u^d \in \mathcal{U}^d : \\ f^d(x^d, p^d, u^d) = 0\},\end{aligned} \tag{3}$$

in which $f^d(x^d, p^d, u^d) = F^d(0, x^d, p^d, u^d)$. The whole set of feasible steady-states is given by the union of all steady-states

$$\mathcal{X}_s^* = \bigcup_{d \in \mathcal{D}} \mathcal{X}_s^{d,*}. \tag{4}$$

In the following the problem of computing an outer-approximation of $\mathcal{X}_s^*$ is considered. This was previously done by Waldherr et al. (2008) for differential equations with polynomial right hand sides. The main contribution of this paper is a generalization of these results to hybrid non-polynomial DAE systems.

3. BOUNDING BY PIECEWISE-POLYNOMIAL FUNCTIONS

The computational method we propose allows to handle uncertain systems that are described by polynomial equations. Therefore, (2) is transformed to a set of uncertain polynomial equations. In the case that f^d is rational, this can be trivially achieved by multiplying with the denominator. In cases in which the systems are non-rational, it is more difficult.

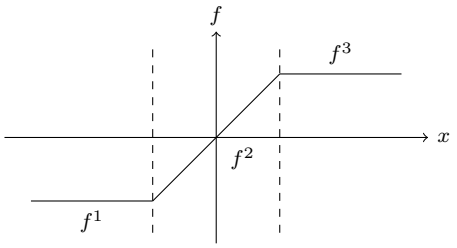

Fig. 1. Saturation function as example for the partitioning of piece-wise polynomial functions.

Savageau and Voit (1987) showed that any system with smooth non-polynomial nonlinearities can be converted to a polynomial system of larger state dimension, which is restricted via equality constraints to a manifold of the dimension of the original system. Unfortunately, in many cases the equality constraints are non-polynomial and so their method is not applicable for our approach. Instead, we apply a different method, which achieves a comparable result without enlarging the state space.

Piece-wise polynomial functions: In case that f^d is piece-wise polynomial, e.g. piece-wise linear, the state space can be partitioned into different intervals. This leads to an increase in the number of decision variables of the hybrid system and is illustrated in Figure 1 for the saturation function, which appears for instance if a process contains flow limiting valves. It has to be emphasized that in cases like this, the partitioning depends on the state. Thus, for a given region in state space $\mathcal{X}$ only a subset of decision variables $d \in \mathcal{D}$ is accessible.

General nonlinear functions: For functions which are not piece-wise polynomial, e.g. the exponential terms in the Arrhenius like rate constant, polynomial lower and upper bounds can be introduced as

$$\begin{aligned} g_1^d(x^d,p^d,u^d) \leq & f^d(x^d,p^d,u^d) \leq g_2^d(x^d,p^d,u^d) \\ & \forall x^d \in \mathcal{X}^d,\ p^d \in \mathcal{P}^d,\ u^d \in \mathcal{U}^d, \end{aligned} \tag{5}$$

in which $\mathcal{X}^d$ is the set in state space of interest. Using these bounds it can be shown that

$$\begin{aligned} \mathcal{X}_s^{d,*} \subseteq \{\ x^d \in \mathbb{R}^{n_x^d} | \exists\ p^d \in \mathcal{P}^d, u^d \in \mathcal{U}^d, c \in [0,1]: \\ c g_1^d(x^d,p^d,u^d) + (1-c) g_2^d(x^d,p^d,u^d) = 0 \} . \end{aligned} \tag{6}$$

Hence, the steady-state constraint $f^d(x^d,p^d,u^d) = 0$ can be substituted by the polynomial constraint

$$c g_1^d(x^d,p^d,u^d) + (1-c) g_2^d(x^d,p^d,u^d) = 0, \quad c \in [0,1], \tag{7}$$

where c has to be appended to p^d. This step corresponds to a constraint relaxation and $||f^d(x^d,p^d,u^d) - g_i^d(x^d,p^d,u^d)|| \ll 1$ should be enforced to keep the difference between $\mathcal{X}_s^{d,*}$ and the set of solutions of the relaxed problem small.

Combinations of the methods, e.g. rational, polynomial and nonlinear functions are possible, see Section 6.

4. BOUNDING STEADY STATES

In this section a method to compute an outer approximation of the state space region containing all steady-states is derived. For this purpose we define the feasibility problem,

$$(P): \begin{cases} \text{find} & d \in \mathcal{D},\ x^d \in \mathbb{R}^{n_x^d}, p^d \in \mathbb{R}^{n_p^d}, u^d \in \mathbb{R}^{n_u^d} \\ \text{subject to} & f^d(x^d,p^d,u^d) = 0 \\ & x^d \in \mathcal{X}^d,\ p^d \in \mathcal{P}^d,\ u^d \in \mathcal{U}^d, \end{cases}$$

which is in the following used for the classification of $\mathcal{X}^d$. If (P) is infeasible, $\mathcal{X}^d$ cannot contain any equilibrium points. (P) is called a mixed integer nonlinear program. Unfortunately, the feasibility problem (P) is in general non-convex and NP-hard.

Kuepfer et al. (2007) proposed a framework for relaxing a polynomial non-convex feasibility problem to a semidefinite program (SDP). Due to inherent convexity of SDPs, these problems can be solved computationally efficient, e.g. via primal-dual interior point methods. In the following, we present an approach which is based on the work of Kuepfer et al. (2007) and has been used for analysis of the set of feasible steady states in the case of biochemical reaction networks in Waldherr et al. (2008).

For the relaxation of (P) to a SDP, the original feasibility problem is at first rewritten as a quadratic feasibility problem (QP), for each d. Therefore, the vectors $\xi^d \in \mathbb{R}^{n_\xi^d}$ are introduced, which consists of the monomials of the model equation (1), i.e.

$$\xi^d = (1,\ x_i^d,\ p_j^d,\ u_k^d,\ x_i^d p_j^d,\ x_i^d u_k^d,\ p_i^d u_k^d, \ldots)^T \tag{8}$$

for all $i \in N_x^d$, $j \in N_p^d$, and $k \in N_u^d$. Using this monome vectors ξ^d, the equality constraints $f^d(x^d,p^d,u^d) = 0$ can be transformed to

$$0 = f_i^d(x^d,p^d,u^d) = \xi^{dT} Q_i^d \xi^d, \quad i \in N_x^d, \tag{9}$$

in which $Q_i \in \mathcal{S}^{n_\xi}$. Note that for higher order terms, additional constraints have to be introduced. For instance if ξ^d contains the second order term $x_1^d p_1^d$, the constraint $x_1^d p_1^d = x_1^d \cdot p_1^d$ must be introduced to express the dependency of the higer order monomial on the first order monomials. This leads to additional constraints of the form,

$$\xi^{dT} Q_i^d \xi^d = 0, \quad i \in N_c^d, \tag{10}$$

in which $Q_i \in \mathcal{S}^{n_\xi}$, $N_c^d = \{n_x^d + 1, \ldots, n_x^d + n_c^d\}$, and n_c^d is the number of dependencies. To simplify the notation we set $N_{xc}^d = N_x^d \cup N_c^d$.

To further simplify the notation we restrict $\mathcal{X}^d$, $\mathcal{P}^d$, and $\mathcal{U}^d$ to be generated by the intersection of half-spaces, e.g. $\mathcal{X}^d$, $\mathcal{P}^d$, and $\mathcal{U}^d$ can be convex polytopes. In this case, $x^d \in \mathcal{X}^d$, $p^d \in \mathcal{P}^d$, and $u^d \in \mathcal{U}^d$ can be written as

$$B^d \xi^d \geq 0, \tag{11}$$

in which $B^d \in \mathbb{R}^{n_b^d \times n_\xi^d}$, and n_b^d is the sum of constraints on x^d, p^d, and u^d.

The original feasibility problem (P) can then be restated as

$$(QP): \begin{cases} \text{find} & \xi^d \in \mathbb{R}^{n_\xi^d},\ d \in \mathcal{D} \\ \text{subject to} & \xi^{dT} Q_i^d \xi^d = 0,\ i \in N_{xc}^d \\ & B^d \xi^d \geq 0 \\ & \xi_1^d = 1. \end{cases}$$

Using the ideas suggested by Parrilo (2003), the (QP) is subsequently relaxed to a SDP, for each d, by introducing the matrices $X^d = \xi^d \xi^{dT}$ and dropping the appearing non-convex constraint $\text{rank}(X^d) = 1$. This leads to the relaxed feasibility problem

$$(RP): \begin{cases} \text{find} & X^d \in \mathcal{S}^{n_\xi^d},\ d \in \mathcal{D} \\ \text{subject to} & \operatorname{tr}(Q_i^d X^d) = 0,\ i \in N_{xc}^d \\ & B^d X^d e_1^d \geq 0 \\ & B^d X^d B^{dT} \geq 0 \\ & \operatorname{tr}(e_1^d e_1^{dT} X^d) = 1 \\ & X^d \succeq 0, \end{cases}$$

in which $e_1^d = (1, 0, \ldots, 0)^T \in \mathbb{R}^{n_\xi^d}$. Note that the relaxation may induce additional solutions. To reduce conservatism, the redundant constraint $B^d X B^{dT} \geq 0$ is added, which is fulfilled by every solution of the problem (QP) (Kuepfer et al., 2007).

From (RP) one can derive the Lagrange dual problem (DP_d) for each d,

$$(DP_d): \begin{cases} \text{maximize} & \nu_1^d \\ \text{subject to} & e_1^d \lambda_1^{dT} B^d + B^{dT} \lambda_1^d e_1^{dT} + B^{dT} \lambda_2^d B^d \\ & + \lambda_3^d + \nu_1^d e_1^d e_1^{dT} + \sum_{i \in N_{xc}^d} \nu_{2,i}^d Q_i^d = 0 \\ & \lambda_1^d \geq 0,\ \lambda_2^d \geq 0,\ \lambda_3^d \succeq 0, \end{cases}$$

in which the Lagrange multipliers are $\lambda_1^d \in \mathbb{R}^{n_b^d}$, $\lambda_2^d \in \mathcal{S}^{n_b^d}$, $\lambda_3^d \in \mathcal{S}^{n_\xi^d}$, $\nu_1^d \in \mathbb{R}$ and $\nu_2^d \in \mathbb{R}^{n_x^d + n_c^d}$ (Waldherr et al., 2008). Using the dual problem, one can obtain an infeasibility certificate for the original problem.

Lemma 2. Let $\nu_1^{d,*}$ be the optimal cost of (DP_d). If

$$\inf \left\{ \nu_1^{d,*} \mid d \in \mathcal{D} \right\} = \infty, \tag{12}$$

then the original feasibility problem (P) is infeasible.

This follows directly from weak duality. Only if the Lagrange dual problem is unbounded from above for all $d \in \mathcal{D}$ the infeasibility of (P) can be guaranteed. The advantage of the formulation using the Lagrange duals is that all subproblems are convex and can be solved efficiently.

In case that $\operatorname{card}(\mathcal{D}) \gg 1$, checking all the distinct combinations of decision variables can become very costly. One possibility to reduce the problem size is to divide $\mathcal{D}$ into subsets $\mathcal{D}_i$. The subsets $\mathcal{D}_i$ can be merged to a common node and the analysis can be performed for all subsets instead of for all nodes. This approach can also be combined with a hierachical refinement of the subsets $\mathcal{D}_i$, which reduces the computational demand significantly.

5. ALGORITHM

Using the Lagrange dual problem (DP_d), certificates for the infeasibility of (4) can be computed. This allows to exploit (DP_d) to determine an outer approximation $\mathcal{X}_s$ of $\mathcal{X}_s^*$. In this work, this is done via simple a multi-dimensional bisection algorithm (Jaulin et al., 2001). Compared to the work by Waldherr et al. (2008) this allows a better approximation of $\mathcal{X}_s^*$ but is computationally more demanding. The basic implementation can be summarized as follows:

Algorithm: $\mathcal{X}_s = \text{Approximation-}\mathcal{X}_s^*(\mathcal{X}, \mathcal{P}, \mathcal{D})$

1. If volume$(\mathcal{X}) < \epsilon$, return $\mathcal{X}_s = \mathcal{X}$
2. Check feasibility of $DP_d(\mathcal{X}, \mathcal{P}, \mathcal{D})$, $\forall d \in \mathcal{D}$
3. If $\inf \left\{ \nu_1^{d,*} \mid d \in \mathcal{D} \right\} = \infty$, return $\mathcal{X}_s = \emptyset$
4. If $\inf \left\{ \nu_1^{d,*} \mid d \in \mathcal{D} \right\} \neq \infty$:
   - 4.1. Bisection of $\mathcal{X}$ in $\mathcal{X}_1$ and $\mathcal{X}_2$
   - 4.2. $\mathcal{X}_{1,s} = \text{Approximation-}\mathcal{X}_s^*(\mathcal{X}_1, \mathcal{P}, \mathcal{D})$
   - 4.3. $\mathcal{X}_{2,s} = \text{Approximation-}\mathcal{X}_s^*(\mathcal{X}_2, \mathcal{P}, \mathcal{D})$
   - 4.4. Return $\mathcal{X}_s = \mathcal{X}_{1,s} \cup \mathcal{X}_{2,s}$

Remark 3. Note that for the application of this algorithm an initial set $\mathcal{X}_0$ must be chosen. If we want to guarantee that an outer approximation of $\mathcal{X}_s^*$ is found containing all feasible equililbrium points, $\mathcal{X}_s^* \subseteq \mathcal{X}_0$ must hold. This is not a restriction because a suitable $\mathcal{X}_0$ can often easily be determined from physical insight into the problem.

6. BOUNDING THE STEADY STATES OF A CSTR

In order to illustrate the proposed scheme the steady-state behavior of a CSTR is analyzed. The reactor considered is a simple tank filled with fluid stirred by an impeller, an inflow and an outflow, as depicted in Figure 2.

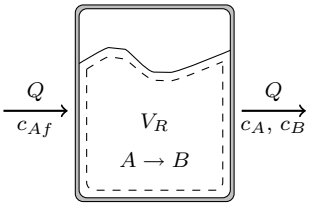

Fig. 2. Schematic of the considered simple CSTR.

6.1 System description

Specifically we consider an adiabatic, constant volume CSTR in which the first-order, exothermal liquid-phase reaction

$$A \xrightarrow{k} B$$

takes place. The conversion rate is given by $R = k(T)c_A$, in which the reaction rate constant is modelled using Arrhenius' equation,

$$k(T) = k_\infty e^{-\frac{E}{RT}}. \tag{13}$$

Simple mass and energy balances lead to the following set of ordinary differential equations:

$$\begin{aligned} \frac{dc_A}{dt} &= \frac{1}{\theta}(c_{Af} - c_A) + k(T)c_A \\ \frac{dT}{dt} &= \frac{1}{\theta}(T_f - T) - \frac{\Delta H_R}{C_p \rho} k(T) c_A, \end{aligned} \tag{14}$$

which captures the dynamics of the CSTR (Rawlings and Ekerdt, 2002). The state variables are the concentration c_A of reactant A, and the reactor temperature T. The parameters are the mean residence time $\theta = V_R/Q$, the reactor volume V_R, the flowrate Q, the concentration of A in the feed stream c_{Af}, the feed stream temperature T_f, the reaction enthalpy ΔH_R, the heat capacity of the fluid C_p, and the fluid density ρ. The numerical values of the nominal parameters are provided in Table 1.

6.2 Analysis of the nominal CSTR

In case that all parameters are known, one can exactly predict how the reactor behaves in different operating conditions. Hereby, since the mean residence time θ is the easiest parameter to manipulate, the operating condition will be defined in terms of θ. The other parameters are assumed to be fixed.

Table 1. Parameter values.

Parameter	Value	Units	Uncertainty
T_f	298	K	3K
C_p	4.0	KJ/kg K	5%
c_{Af}	2.0	kmol/m^3	5%
k_∞	5.0×10^8	min^{-1}	5%
E/R	8.0×10^3	K	–
ρ	10^3	kg/m^3	–
ΔH_R	-3.0×10^5	kJ/kmol	5%

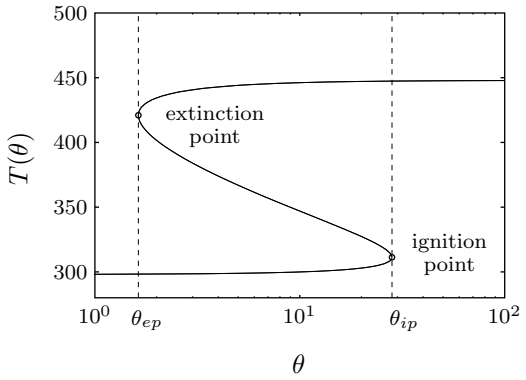

Fig. 3. Bifurcation diagram of CSTR without parameter uncertainties.

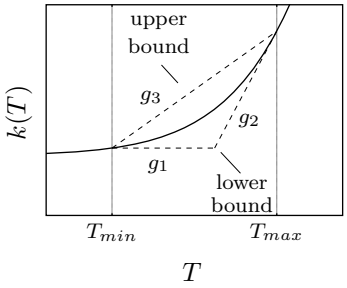

Fig. 4. Bounding of $(-)$ Arrenhius term with $(--)$ linear functions.

Using continuation methods it is possible to numerically compute the steady-state curve (bifuraction diagramm) for varying residence times (Dhooge et al., 2003), as shown in Figure 3. θ_{ep} and θ_{ip} denote the mean residence time at the extinction and the ignition point respectively.

6.3 Analysis of CSTR with parameter uncertainties

If one or more parameters are uncertain, which is in practice always the case, calculating the set of steady-state is significantly more challenging. Typically, sampling based techniques such as Monte-Carlo like methods are used. These allow the approximation of the union of all feasible equilibrium points $\mathcal{X}_s^*$. However, as for all Monte-Carlo like methods no bounds for the obtained sets can be provided. Our approach overcomes this problem and enables us to compute an outer approximation of the set of feasible equilibrium points of the uncertain system.

Approximation of the rate constant: Applying the proposed method requires in a first step to bound the Arrhenius-like rate constant from below and from above using polynomial functions. In this paper $k(T)$ is bounded via three linear functions,

$$\max(g_1, g_2) \leq k \leq g_3, \quad \forall T \in [T_{min}, T_{max}], \tag{15}$$

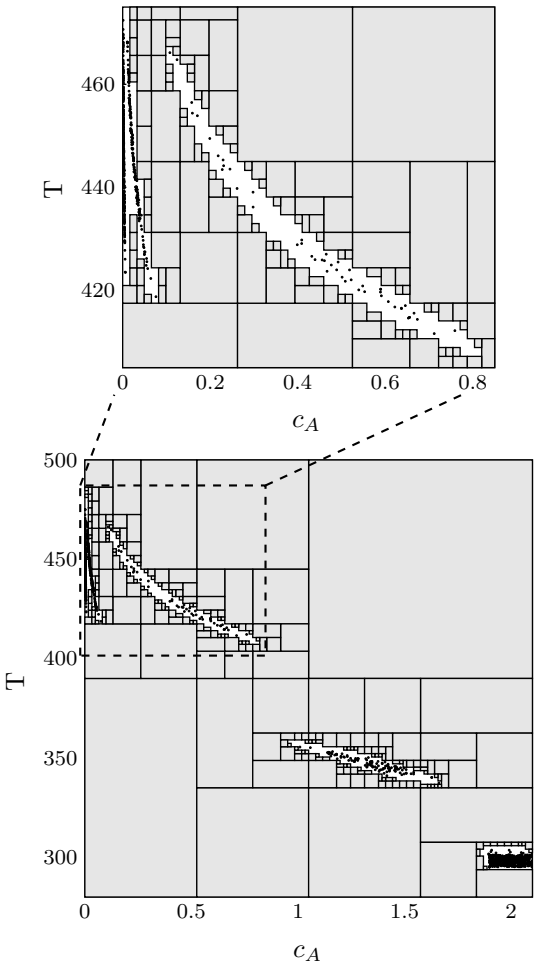

Fig. 5. Region in state space which cannot contain steady-states for given parameter uncertainties and $\theta \in \{1, 10, 100\}$ versus $(\cdot)$ steady-states computed using Monte-Carlo sampling.

as depicted in Figure 4. This approach is very simple and has the disadvantage that the approximation of $k(T)$ is less precise if the difference of T_{min} and T_{max} becomes large. Therefore, we don't use a static approximation but rather select g_1, g_2 and g_3 in each interation of the bisection algorithm dependent on the box $\mathcal{X}$ in state space currently under consideration. This allows to keep the overestimation of the set of feasible steady-states small as will be seen later.

One could of course choose other methods to bound $k(T)$, for instance based on high order polynomials and the Taylor series expansion, but in many cases the computational effort to solve the semidefinite program once will increase significantly and the presented simplistic approach will be more efficient.

Set of feasible steady-states: The above derived theory and the bounding of $k(T)$ allow to compute the set of feasible steady-states of the CSTR. As decision variable we consider besides the temperature interval also the mean residence time θ. Additionally, most parameters are uncertain. The amounts of uncertainty with respect to the nominal values are provided in Table 1.

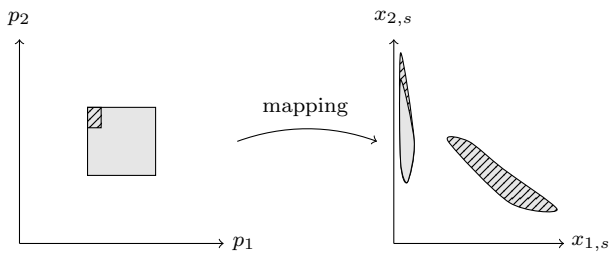

Fig. 6. Illustration of the nonlinear mapping from parameter to steady-states.

The algorithm outlined in Section 5 is in the following used to estimate the set of all feasible equilibrium points of (14) for the given parameter uncertainties and $\theta \in \{1, 10, 100\}$. The results are shown in Figure 5, where the part of the state space which is certified infeasible is marked light gray. To compare our results with classical approaches, five thousand equally distributed Monte-Carlo samples for the accessible parameter set were taken and the steady-states were determined.

Computation of the set of feasible steady-states: As one can see, the results match with each other. However, a closer look at the results reveals several disadvantages of the sampling based approach. First of all, the number of samples in some regions of the state space is small compared to other regions, where the sampling density is extremely high. This indicates that many parameters lead to steady-states in the region with high sampling density, but there are still some regions that cannot be explored unless even higher numbers of samples are used. This might represent a problem, whenever the set of all feasible steady-states has to be computed, since normally a homogeneous sampling rate is more desireable. However, the Monte-Carlo method is not able to guarantee under such a condition that the whole state space is explored, due to the highly nonlinear mapping between parameters and steady-states, illustrated in Figure 6. Therefore, the set of feasible equilibrium points is always underestimated, even for exhaustive Monte-Carlo sampling, while the proposed method guarantees that all equilibrium points are contained in the determined set.

7. CONCLUSION

In this work we studied the problem of outer bounding the region in state space containing all equilibrium points of uncertain hybrid differential algebraic systems. The proposed method is based on the formulation as a feasibility problem and a relaxation to a SDP. It is shown that guaranteed outer bounds of the feasible set of equilibrium points can be determined.

The advantage of the proposed methodology in comparison to Monte-Carlo based approaches is explained and shown considering a simple CSTR process. In particular, the developed method does not rely on sampling and can deal with strongly nonlinear and non-unique mappings from parameters to steady-states.

The computed set is guaranteed to contain all feasible steady-states, thus worst case scenarios can be analyzed. This is of certain interest to evaluate controller performance in fault situations.

8. ACKNOWLEDGEMENTS

This work was supported by the Forschungseinheiten der Systembiologie (FORSYS) [grant 0315280D]; the International Max Planck Research School Magdeburg; and by the Stuttgart Research Centre for Simulation Technology.

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