Scenario-Integrated Modeling and Optimization of Dynamic Systems

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Assessing the consequences of exceptional events, such as failures and sudden changes in product demand or raw-material prices, is of great importance to the operation of chemical processes. Such an exceptional event and the resulting behavior of the process are called a scenario in this article. Problem formulations for their rigorous incorporation into the optimization of dynamic systems are presented. They allow the determination of operational strategies that are economically optimal and that keep the plant within a chosen regime in the state space, even for a number of possible scenarios. The formulations are based on a unifying model framework containing both continuous and discrete dynamics. For a restricted class of problems a method for the numerical solution of the resulting scenario-integrated dynamic optimization problems is introduced. The applicability of this technique is demonstrated with two examples of different complexity.

Introduction

The simulation of dynamic systems has emerged from a pure research discipline to a standard method for designing and studying operational strategies in the chemical-process industries (Marquardt, 1991). Today, commercial tools such as SPEEDUP, gPROMS, and ABACUSS are available to deal with thousands of equations, thus allowing the treatment of a wide variety of chemical processes. Dynamic simulation naturally deals with processes that are operated in transient phases. Notable examples include batch and semibatch reactors as well as continuous processes under periodic excitation or during grade changes, startup, and shutdown.

When industrial case studies dealing with dynamic simulation are analyzed, two interesting observations can be made. The first observation is that, in many cases, the focus of the corresponding engineering projects is often not to simply describe the conventional operation of the processes, but to find optimal, or at least improved, operational strategies. This aim is usually achieved by performing a large number of successive simulations using different input functions. More systematically, such a task is formulated as a dynamic optimization problem. The numerical solution of these problems is currently an active area of research (Biegler, 1998; Feehery and Barton, 1998; Schulz et al., 1998). Mature and reliable techniques can be expected to be available, also commercially in the future. The second observation is that often the effect of uncertainties on the system behavior is investigated. These situations may either arise from expected changes in the external environment of the system or from events within the system itself. Examples include changing market prices or weather conditions for the former and equipment failures for the latter case. Here we call such a hypothetical situation initiated at a specific time instant a *scenario*.

These two observations prompt the question whether the treatment of scenarios and the optimization of dynamic systems could be combined to provide an integrated design procedure. Such an approach has already been suggested for cases where only parametric uncertainties exist. The resulting technique is called *robust optimization* (Terwiesch et al., 1994). The uncertain parameters are here assumed to remain constant over the time period of interest. This assumption is not always justified. First, the uncertainties considered may not only affect model parameters but might also influence the structure of the stated process model. Second, uncertain variables may also change their values during the course of the process. Among the various possibilities of how these variabilities might appear, for the purposes of this article, we restrict ourselves to the special case of instantaneous changes. The system response to these changes does not only depend on the modified variable values in these cases, but also on

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the specific time instants at which the changes occur. This introduces specific problems for the optimization of dynamic systems that will be analyzed in the present work. Several classes of dynamic optimization problems are discussed based on new model framework for the integration of scenarios into the treatment of transient processes. A first numerical solution approach for a restricted subclass of the formulated problems is developed.

Scenario-integrated modeling and optimization of dynamic systems is related to a number of research areas. In order to be able to adequately illustrate the similarities and the differences between these areas and the approach proposed in this article, we leave any further survey of the literature for later sections. Instead, in the following section, we start by discussing a number of motivating examples, from which we extract common characteristics. Two major problem areas are introduced that differ in the nature of the scenarios and objectives to be achieved therein. The suggested scenario-integrated modeling framework for dynamic systems is presented in the third section. Since the start of a particular scenario is treated as a discrete event, this model is based on a hybrid (discrete-continuous) system representation. At the start of the event, the system switches from one discrete mode to another. The derived framework enables us in the fourth section to elaborate mathematically the scenario-integrated optimization problems for dynamic systems. As will be shown, all problem formulations are of infinite dimensionality in various aspects, such that numerical solutions can only be achieved in an approximate sense. One possibility for approximating these problems, which allows the application of existing numerical techniques, is discussed in the fifth section. Finally, the formulation and solution of scenario-integrated dynamic optimization problems are illustrated in the sixth section by considering two examples, where safety constraints are enforced despite failures.

Motivating Examples

Optimization under uncertainty, also called *stochastic optimization*, is an established research discipline that attempts to find optimal decision variables when certain parts of the problem formulation cannot be described deterministically. Most of the work that has been performed in the past is restricted to the treatment of stationary processes where some of the model parameters are unknown (Birge and Louveaux, 1997; Darlington et al., 1999). A probability density function of the unknown parameters is often assumed to be available. In this case, various objectives can be used, such as the minimization of the expected cost, the minimization of the cost variance, and the minimization for the worst parameter values. In the first two cases integral expressions over the uncertainty domain have to be evaluated in the objective functions. Most frequently, these integrals cannot be solved analytically, so some approximation must be introduced. A common approach is to sample the probability distribution by a finite number of parameter values. These samples of the stochastic process are viewed as possible scenarios.

Many of these approaches can be generalized to the treatment of dynamic systems that are subject to unknown parameters. Since the probability distributions for these parameters are usually assumed to remain constant over time, the optimization is now subject to a stationary stochastic process. With emphasis on the minimization of the expected cost, this case has been extensively studied in the past (Mohideen et al., 1996; Terwiesch et al., 1994). The operational degrees of freedom are time varying here, and the resulting problems therefore show an infinite dimensionality not only with respect to the parameter values but also with respect to the decision variables. In order to apply conventional dynamic optimization techniques, the probability density functions for the parameters are again discretized, and only a finite number of sample parameter values is considered.

An obvious extension of this type of optimization problem under uncertainty is to allow parameter changes at arbitrary instants over the time period of interest. Since the number of possible instants is again infinite, a third level of complexity is added. In the past, this difficulty was tackled by the same approach that was used for the previous dimensionality problems. Thus, the time coordinate is discretized and the optimization problems to be solved are formulated in discrete time only. The instants considered are called *stages* where the uncertain parameters can use values from a discretized probability distribution. This leads to a scenario tree of possible parameter values over time. The optimization problems are therefore subject to completely discretized systems that support stationary as well as unstationary stochastics. The resulting formulations are commonly called multistage stochastic programming problems (Infanger, 1994; Rockafellar and Wetts, 1991). They are further illustrated by the following examples.

Example 1: Production Planning in a Transient Business Environment. In order to operate plants optimally, production is usually forecast for a certain time period. The market prices of the raw materials and the assumed customer demand for the produced substances are the input variables for these planning problems. Unfortunately, the prediction of these parameters is often affected by major uncertainties about market and consumer behavior. First, it is unknown whether any deviation from the nominal values will be observed. If such a deviation is assumed to occur, it is unknown when it will start and to what extent the variables will differ from their nominal values. A representative case study for problems dealing with electrical power generation is presented by Nowak and Römisch (1998).

Multistage stochastic programming approaches are mainly used for planning problems in operations research. They are, however, equally suited for situations related more to operational questions, such as is outlined by Example 2:

Example 2: Batch Distillation Column. Batch distillation columns are often operated at temperatures that are significantly different from the ambient temperature. Since the heat exchange with the environment depends on the existing temperature difference, the quality of the distillate can suffer from sudden changes in the ambient conditions if the time-varying operational strategy is not appropriately adapted. For example, such a sudden change in the ambient conditions results from cold rain on a hot day. Again it may be unknown if the weather conditions will indeed change. If they change, the instant at which the rain will start, as well as the associated temperature decrease, are unknown.

These problems are always of combinatorial complexity. For only a single uncertain parameter with n samples parameter values and k stages over time, the number of possible scenarios is already n^k. The economic objective used has now to be evaluated for all n^k scenarios distinguished by n^k different parameter values. In order to obtain a single objective function to be minimized, several possibilities exist. In most cases, an expected value formulation is used where the different objective functions are weighted by the probability of the scenarios and summed. The solution of a multistage stochastic programming problem then provides a single operational strategy that is robust against the considered parametric uncertainties.

More general approaches are desirable for many problems related to the optimal operation of chemical processes under uncertainty. These approaches should be able to cope with changes that not only influence certain parameters but that also affect the structure of the process. Furthermore, the determination of one single operational strategy is inappropriate if the changes can be easily detected. This situation holds for uncertain prices and customer demands in Example 1, as well as for the measurable ambient temperature in Example 2. The available information on these variables can be exploited in order to push the processes closer to the achievable economic optimum by appropriately changing the operational strategy. Sometimes, such an adaptation is not only economically desirable but even necessary in order to ensure that the existing constraints are fulfilled for the time after the changes. This is illustrated by the following two examples dealing with highly exothermic semibatch reactors:

Example 3: Semibatch Reactor with Partial Cooling-System Failure. In the operation of highly exothermic semibatch reactors multiple cooling systems are sometimes used (Collins et al., 1997). One part of the cooling system often consists of a jacket around the reactor, and a second part is provided by a coil in the vessel. If one of these cooling systems fails during a batch, the feed flow rate to the reactor and the cooling strategy of the remaining system must be changed in order to ensure the feasibility of the existing constraints and to ultimately save the batch to the extent possible.

Example 4: Two-Phase Semibatch Reactor with Stirrer Failure. In order to ensure that the raw materials react sufficiently well with the substances in the vessel, the contents of semi-batch reactors are usually stirred, thus creating approximately the same conditions in all parts of the reactor. If one of the reactants is found predominantly in the vapor phase, additional "stirring" is often achieved by the dispersion of gas bubbles into the reactor. If the stirrer motor fails, the assumption of a perfectly mixed reaction system is less justified. Areas with slow reaction can then be distinguished from areas with fast reaction. However, the batch might still be operated to the defined endpoint if the trajectories of the feed flow rate and the desired temperature are adapted appropriately.

Obviously, an adaptation of the operational strategies is necessary in these cases in order to prevent a dangerous violation of existing safety constraints. Furthermore, these examples clearly support the requirement for different model structures. For instance, in Example 3 the failed cooling system can be eliminated from the model used after the failure. In contrast, the assumption of an ideally stirred system might no longer be justified after the failure in Example 4. Here, a model reflecting the imperfect mixing situation, for example a cell model, would have to be formulated. This results in a far more complicated equation system than is used for the description of the nominal operation.

The optimization approaches developed in this article are specifically tailored to these characteristics. Two subclasses are hereby delineated. In the first, the nature of the scenarios and the operational goals favor the use of the same economic objective function independently of any change or event that might happen during the transient process. The various process phases all contribute to the same overall objective function such that this class will be called *single-level scenario-integrated optimization problems*. All examples discussed so far belong to this paradigm. It must be seen as an extension of multistage stochastic programming problems. For the purposes of this article we restrict the uncertainties to unknown event time instants, assuming a perfect process model to be available during the nominal operation and for the scenarios considered. The complexity is further reduced by assuming a uniform distribution for the uncertain time instants, which is realistic, particularly for those cases where the amount of statistical data is insufficient for more detailed descriptions.

The second subclass of optimization problems discussed in this article does not assume that the same economic objective function is applied for the nominal operation and in the scenarios. Instead, we suppose here that an economic optimization is performed for the nominal operation only, and that secondary goals exist for the scenarios. An example for this situation is easily constructed:

Example 3 Reconsidered: Semibatch Reactor. Sometimes emergency rules might suggest that the process be shut down after the loss of the cooling system, preventing any further economic optimization. The time to reach operating conditions characterized by low temperatures and pressures might then be used as a secondary goal for the time after the failure.

Here, the available degrees of freedom are used to minimize two different objective functions where only one is related to economics. A variant of this problem results if the considered scenario does no longer contain any operational degrees of freedom. The formulation of secondary goals then becomes useless and only constraints have to be enforced in the scenarios. Obviously, this can only be achieved by an appropriate choice of operational degrees of freedom during the nominal operation. Several examples of this problem type can be found in the literature:

Example 5: Car Problem with Brake Failure (Abel et al., 1998). In this example a car with possibly malfunctioning brakes is traveling on a road that ends in front of a wall. The objective is to cover a fixed distance in the minimum time. An operational strategy has to be chosen such that the car does not hit the wall even in the case where the brakes fail and only friction effects decelerate the car. Acceleration would make the situation even worse, and can be excluded *a priori*. Thus, no degrees of freedom are left after the brake failure and only the endpoint has to be investigated.

Example 6: Semibatch Reactor with Total Cooling System Failure. In principle, the same situation holds for an exothermic semibatch reactor where only one cooling system exists that might fail during the batch. Still, feeding educts to the reactor after a cooling-system failure would increase the energy potential and does not have to be considered. If an inhibitor or an emergency cooling system does not exist, the temperature and the pressure in the reactor rise. In that case, the operational strategy in the nominal mode must already be chosen such that critical limits are not exceeded after the failure (Gygax, 1988; Stoessel, 1995).

The main feature of the optimization problems formulated for these examples is their layered structure. We will therefore refer to them as *bilevel* (or *multilevel*) *scenario-integrated optimization problems*. Economic optimization is carried out only for nominal operation. Depending on the number of available degrees of freedom, the subproblem minimizes secondary goals or reduces to a feasibility test. Similar problems have been formulated in the past in the area of bilevel programming (Cheng and Florian, 1995; Falk and Liu, 1995). To the authors' knowledge, a fully dynamic analog of these problems is formulated here for the first time. Although the single-level problems introduced earlier and the bilevel problems discussed here are different with respect to their optimization structure, they share the common characteristics that specific operational profiles are determined for possible scenarios and that different process models can be used during nominal operation and the scenarios. Both classes are therefore called *scenario-integrated optimization problems*.

Scenario-Integrated Modeling of Dynamic Systems

As discussed in the previous section, the phenomena initiating a scenario usually occur on a much shorter time scale than the nominal dynamics of the chemical processes considered. We therefore assume that these changes can be described by an instantaneous event. The resulting discrete elements render the scenario-integrated model description of a hybrid (discrete-continuous) nature. Hybrid systems have attracted much interest in the recent literature (Alur et al., 1995; Barton and Pantelides, 1994; Benveniste, 1996; Nerode and Kohn, 1993; Nicollin et al., 1993), and the main achievements in their modeling and control have been summarized in two recent reviews (Barton and Park, 1997; Engell et al., 1997). The scenario-integrated model formulation suggested here is based on these descriptions, which are therefore briefly reviewed in the following subsection.

Hybrid systems

Two approaches to a mathematical formulation of hybrid systems are often delineated. In one line of research continuous models have been generalized by incorporating discrete events (Barton and Pantelides, 1994; Branicky et al., 1998; Tavernini, 1987). This view has been commonly taken in process systems engineering where applications typically show a continuous part consisting of a large set of differential-algebraic equations (DAE) and a comparatively small discrete part. A second concept for the modeling of hybrid systems originated in the purely discrete world of finite automata. It describes the behavior of the system in the discrete states by using differential equations to result in the so-called hybrid automata (Alur et al., 1995; Nicollin et al., 1993). Here, the focus has been on dealing with a comparatively large discrete subsystem while putting less emphasis on the continuous part. The latter is often only described by a number of linear ordinary differential equations (ODEs). For the purpose of this article, the differences between these approaches are subtle.

For the proper definition of a hybrid system three issues have to be tackled (Barton and Park, 1997): the continuous part, the discrete part, and their mutual interaction. Generally, the discrete part of the system is simply captured by a variable $\xi \in \Xi$ indicating the *mode* of the hybrid system. The modes are often numbered in ascending order $\Xi = \{0, 1, \ldots\}$. (Sometimes ξ is also called the (discrete) *state* of the hybrid system. In order to clearly distinguish the discrete part of the system from the continuous one, the term *state* will be restricted to the continuous variables here and the term *mode* is used to refer to the discrete part of the hybrid system.) The continuous part is conveniently described by the DAE

$$0 = f_{\xi}\left(\dot{x}_{\xi}, x_{\xi}, y_{\xi}, u_{\xi}, t\right) \tag{1}$$

for each discrete mode ξ. Here, $t \epsilon T = [t_0, t_f] \subset \mathbb{R}$ is the process time interval ranging from the initial time t_0 to the final time t_f; $x_{\xi} \in \mathbb{R}^{n_{\xi}}$ denotes the differential and $y_{\xi} \in \mathbb{R}^{m_{\xi}}$ the algebraic variables that together determine the continuous *state* of the hybrid system; $u_{\xi} \in \mathbb{R}^{p_{\xi}}$ are control variables. They are viewed as design or operational degrees of freedom that need to be fixed in order to determine Eq. 1. The vector function $f_{\xi} : \mathbb{R}^{n_{\xi}} \times \mathbb{R}^{n_{\xi}} \times \mathbb{R}^{m_{\xi}} \times \mathbb{R}^{p_{\xi}} \times \mathbb{R} \to \mathbb{R}^{n_{\xi}+m_{\xi}}$ represents the process model. The number and the type of the model equations f_{ξ} are specific to the discrete modes and may change between subsequent modes. Consequently, the number of differential variables n_{ξ}, the number of algebraic variables m_{ξ}, as well as the number of operational variables p_{ξ} may also change when the mode of the system switches from ξ_i to ξ_j. Without loss of generality it can be assumed in the sequel that the mode of the system at t_0 is enumerated zero, $\xi(t_0) = 0$.

In order to fully specify Eq. 1 for $\xi = 0$, a number of initial conditions have to be stated at t_0. For general DAEs this is not trivial (Pantelides, 1988; Unger et al., 1995) and usually imposes hidden constraints such that the number of dynamic initial conditions at t_0 is smaller than n_0. However, most of the applications in process systems engineering can be modeled as a semiexplicit DAE of the type

$$B_{\xi}(x_{\xi}, y_{\xi}, u_{\xi})\dot{x}_{\xi} = f_{\xi}^{d}(x_{\xi}, y_{\xi}, u_{\xi}), \tag{2}$$

$$0 = f_{\xi}^{a}(x_{\xi}, y_{\xi}, u_{\xi}), \tag{3}$$

where the matrices B_{ξ} and $\partial f_{\xi}^{a}/\partial y_{\xi}$ are square and of full rank. These systems belong to the class of DAEs of index one (Brenan et al., 1996) and require exactly n_0 initial conditions at t_0, which are called the dynamic degrees of freedom (Unger et al., 1995). One possibility for the selection of these degrees of freedom is to fix the differential variables $x_0(t_0)$:

$$x_0(t_0) = x_{0,0}. \tag{4}$$

The initial values of the algebraic variables $y_0(t_0)$ are then calculated from Eq. 3. Although the focus of this article is restricted to these semiexplicit DAEs, the formulation of Eq. 1 will be further used to simplify the notation.

Switching from one mode of the hybrid system ξ_i to another mode ξ_j is modeled by the characterization of a *transition*. This characterization comprises the initial mode ξ_i, the final mode ξ_j, a logical condition triggering the occurrence of the transition, and a mapping between the continuous state variables of modes ξ_i and ξ_j. The logical condition can be expressed mathematically as

$$l_{\xi_i,\xi_j}\left(x_{\xi_i}, y_{\xi_i}, u_{\xi_i}, t\right) = \begin{cases} \leq 0 & \text{if the mode remains to be } \xi_i, \\ > 0 & \text{if the mode changes to } \xi_j, \end{cases} \tag{5}$$

with $l_{\xi_i,\xi_j}: \mathbb{R}^{n_{\xi_i}} \times \mathbb{R}^{m_{\xi_i}} \times \mathbb{R}^{p_{\xi_i}} \times \mathbb{R} \rightarrow \mathbb{R}$ for every possible transition between two discrete modes. The sign of l_{ξ_i,ξ_j} switches if a corresponding logical condition changes its binary value. Another approach would be to construct a function $\bar{l}_{\xi_i,\xi_j}$ to map the continuous state, the operational degrees of freedom, and the time to the binary set $\mathbb{B} = \{0,1\}$ (Barton and Pantelides, 1994; Dimitriadis et al., 1997). Both techniques are able to model composite and complicated switching conditions. Typical examples for such conditions include the case when the continuous system autonomously reaches a boundary of a particular state-space partition. Furthermore, a change of the sign in l_{ξ_i,ξ_j} may simply be triggered by one of the external inputs u_ξ, possibly driven by a controller forcing the system to switch.

Under the assumption that switching between two discrete modes occurs instantaneously at a time $t^*_{\xi_i,\xi_j}$, the mapping of the state variables at a transition can be described by the equation

$$0 = h_{\xi_i,\xi_j}\left(x_{\xi_i}, y_{\xi_i}, u_{\xi_i}, x_{\xi_j}, y_{\xi_j}, u_{\xi_j}, t^*_{\xi_i,\xi_j}\right), \tag{6}$$

with $h_{\xi_i,\xi_j}: \mathbb{R}^{n_{\xi_i}} \times \mathbb{R}^{m_{\xi_i}} \times \mathbb{R}^{p_{\xi_i}} \times \mathbb{R}^{n_{\xi_j}} \times \mathbb{R}^{m_{\xi_j}} \times \mathbb{R}^{p_{\xi_j}} \times \mathbb{R} \rightarrow \mathbb{R}^{n_{\xi_j}}$ for DAEs of index one. Equation 6 implicitly defines n_{ξ_j} specifications at the time instant $t^*_{\xi_i,\xi_j}$ for Eq. 1 in mode ξ_j. One possibility is to state h_{ξ_i,ξ_j} such that, as in the initial mode $\xi = 0$, the values of the differential state variables $x_{\xi_j}(t^*_{\xi_i,\xi_j})$ can be determined from Eq. 6. The algebraic variables $y_{\xi_j}(t^*_{\xi_i,\xi_j})$ are then calculated from Eq. 3. Hence, the algebraic variables can be eliminated in Eq. 6 to result in:

$$0 = h_{\xi_i,\xi_j}\left(x_{\xi_i}, u_{\xi_i}, x_{\xi_j}, u_{\xi_j}, t^*_{\xi_i,\xi_j}\right). \tag{7}$$

Note that this formulation supports continuity, jumps, and impulses of the differential state variables across the discontinuity.

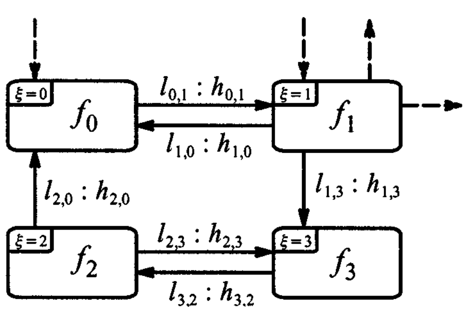

Figure 1. Example of a hybrid system.

An example of a hybrid model formulated in the framework of Eqs. 1 to 7 is illustrated in Figure 1. By definition, the system initially resides in the discrete mode $\xi = 0$. As soon as the logical condition $l_{0,1}$ becomes true the system switches to the mode $\xi = 1$, with an initial value $x_1(t^*_{0,1})$ determined through $h_{0,1}$. Later, the system might switch back to the previous mode $\xi = 0$, move forward to mode $\xi = 3$, or even proceed to other modes indicated in Figure 1 by the dashed lines, leaving the mode $\xi = 1$.

Scenario-integrated modeling with a single transition

The theory of hybrid systems provides a convenient basis for the development of scenario-integrated models for dynamic systems. In order to keep the complexity limited we will first restrict ourselves to the treatment of those systems that can reside in the nominal mode or in a single scenario mode before extending the results to more complicated cases in the following subsection.

Without loss of generality it is assumed that $\xi = 0$ and $\xi = 1$ are associated with the nominal and the scenario mode, respectively. At the start of the scenario, the system switches instantaneously from mode $\xi = 0$ to mode $\xi = 1$. Since only one single transition is allowed here, a switch back to the nominal mode is excluded and the system will stay within the scenario mode $\xi = 1$ for the rest of the time period of interest. This situation arises in particular for failure cases such as illustrated by Examples 3 to 6, where the failed parts of the plant can usually not be repaired during the transient phase of the system. In contrast to more general hybrid systems, the transition between modes is always monodirectional.

Based on the discussion of the examples, it can be concluded that the logical condition $l_{0,1}$ is not influenced by either the state or the control variables in the nominal mode. Hence, in contrast to Eq. 5, $l_{0,1}$ is simply a function of time:

$$l_{0,1}(t) = t - t^*_{0,1}. \tag{8}$$

The switching time $t^*_{0,1}$ is uncertain and can adopt any value in $[t_0, t_f]$. This uncertainty in the logical condition $l_{0,1}$ introduces a major difference between commonly stated hybrid models and scenario-integrated models studied here. In the former class, the model equations, the logical conditions, and the mapping functions can always be solved sequentially starting from the initial time t_0. This leads to a unique discrete mode and to unique values of the state variables for any moment $t \in [t_0, t_f]$. In the latter class, the discrete mode of the system at one particular t depends on the value of the unknown switching time $t^*_{0,1}$. For $t^*_{0,1} > t$, the system is still in the nominal mode, whereas it has already switched to the scenario mode if $t^*_{0,1}$ is smaller than t. Since any instant in the interval $[t_0, t_f]$ is a possible candidate for the switching time $t^*_{0,1}$, the system has to be examined in both modes at all possible times.

At a first glance it might be tempting to capture the uncertainty in the switching time by an appropriate probability density function. This would lead to the formalism of stochastic hybrid systems, a theory that has been developed as an extension of stochastic discrete processes. The best known example of this class is the generalized Markov decision process (Glynn, 1989; Puterman, 1994), which also leads to undetermined modes for a particular moment. Probabilities are then calculated for the system to reside in each of the possible modes. For many practical cases the necessary probability description is difficult to obtain, however, due to the absence of sufficient data. In particular, this holds for the failure situations illustrated earlier in a number of examples in the second section. We therefore prefer to treat the problem in a deterministic setting and allow the system to switch to the scenario mode at any instant with equal probability.

In order to derive a formal description of scenario integrated models of dynamic systems that emphasize the nonuniqueness of the discrete mode, different time axes are introduced. In the sequel, t_0 denotes the time axis of the nominal mode, ranging from the initial time $t_{0,0}$ to the final time of the nominal mode $t_{0,f}$. Within the scenario mode, the system is described along another time axis t_1, which starts at the switching time $t^*_{0,1}$ and ends at the final time of the scenario mode $t_{1,f}$. Depending on $t^*_{0,1}$, different initial conditions $x_1(t_1 = t^*_{0,1})$ are generally determined by the mapping function $h_{0,1}$. Thus, the complete trajectories of the continuous state variables also depend on the switching time: $x_1 = x_1(t_1, t^*_{0,1})$. Since the final time of the system is often defined on the basis of certain values of the continuous state variables, the same dependency holds for the final time in the scenario mode: $t_{1,f} = t_{1,f}(t^*_{0,1})$. In order to keep the notation simple, however, we will, omit the switching time as argument of these variables in the sequel. Retaining the possibility of using different process models in the nominal and the scenario mode, a first scenario-integrated model of dynamic systems can be formulated as

$$
\begin{aligned}
&0 = f_0(\dot{x}_0, x_0, y_0, u_0, t_0),\\
&0 = x_0(t_{0,0}) - x_{0,0},\\
&\qquad \forall t_0 \epsilon \left[t_{0,0}, t_{0,f}\right],\\
&0 = f_1(\dot{x}_1, x_1, y_1, u_1, t_1),\\
&0 = h_{0,1}(x_0, u_0, x_1, u_1, t^*_{0,1}),\\
&\qquad \forall t_1 \in \left[t^*_{0,1}, t_{1,f}\right],\\
&\qquad \forall t^*_{0,1} \in \left[t_{0,0}, t_{0,f}\right].
\end{aligned}
\tag{SIM1}
$$

The specific feature of this formulation is that the event instant $t^*_{0,1}$ can adopt *any* value within the time horizon of the nominal mode $[t_{0,0}, t_{0,f}]$. The analysis of a dynamic system with an incorporated scenario has therefore to cope with an infinite number of switching times from the nominal to the scenario mode. Consequently, the set of all possible trajectories for one specific state variable x forms a surface in the t_0-t_1-x space. This is illustrated in Figure 2. On the time axis t_0, f_0 captures the behavior of the system with the initial conditions given by $x_{0,0}$. The corresponding trajectory $x_0(t_0)$ is plotted by the bold line. At each instant of this trajectory, the system may switch to the scenario mode. For the case shown in Figure 2, the function $h_{0,1}$ has been assumed to consist of the continuity equation $x_0(t^*_{0,1}) = x_1(t^*_{0,1})$ such that the value of the state variable at the switching times remains

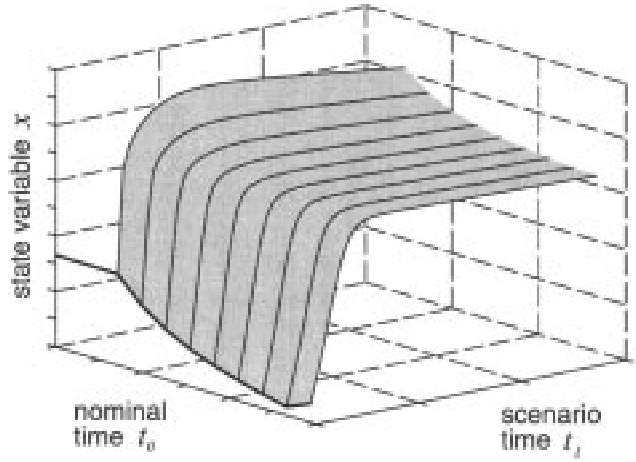

Figure 2. Solution of a scenario-integrated dynamic system.

unchanged. Beginning at these switching times, the process is observed along the time axis t_1 where f_1 describes the system behavior until the final time $t_{1,f}$ is reached. The surface built by all possible trajectories in the scenario mode is indicated by the gray area.

Scenario-integrated modeling with multiple transitions

Although the analysis of dynamic systems with only one incorporated scenario mode is already significantly more complicated than the treatment of conventional dynamic systems, it is desirable to extend the model formulation derived in the preceding subsection to cases with multiple transitions. This is relatively straightforward as long as these transitions are restricted to depart only from the nominal mode. They may then proceed to one out of several scenario modes. This situation only increases the number of possible scenarios to be treated on a single scenario level and therefore does not increase the problem complexity qualitatively. Mathematically, an appropriate formulation can be directly derived from Model SIM1:

$$
\begin{aligned}
&0 = f_0(\dot{x}_0, x_0, y_0, u_0, t_0),\\
&0 = x_0(t_{0,0}) - x_{0,0},\\
&\qquad \forall t_0 \in \left[t_{0,0}, t_{0,f}\right],\\
&0 = f_\xi(\dot{x}_\xi, x_\xi, y_\xi, u_\xi, t_\xi),\\
&0 = h_{0,\xi}(x_0, u_0, x_\xi, u_\xi, t^*_{0,\xi}),\\
&\qquad \forall t_\xi \in \left[t^*_{0,\xi}, t_{\xi,f}\right],\\
&\qquad \forall t^*_{0,\xi} \in \left[t_{0,0}, t_{0,f}\right],\\
&\qquad \xi = 1, \ldots, N.
\end{aligned}
\tag{SIM2}
$$

Here, N scenario modes have been taken into account. The transition to each of the scenario modes is possible for any instant of the nominal mode $[t_{0,0}, t_{0,f}]$, and the scenario-integrated Model SIM2 has to be analyzed on multiple surfaces, each of the type depicted in Figure 2. Including the nominal mode, this results in an investigation along $N+1$ time axes.

Far more challenging than this direct extension of the problem formulation derived in the preceding subsection is the treatment of dynamic systems that do not only switch from a nominal to a scenario mode, but that may also leave a certain scenario mode to switch to another. With each transition the system reaches a mode on a new level. The resulting scenario tree is given in Figure 3. In contrast to commonly stated hybrid systems, the scenario tree has the disadvantage that a new level of discrete modes has to be constructed even if the dynamic system actually switches back to a previously visited mode. On the other hand, the scenario tree provides the advantage of preserving the clear monodirectional motion of the system through the discrete structure. Consequently, the development of an appropriate mathematical problem description can be achieved comparatively easily on the basis of Model SIM2.

The first step towards a formulation of this situation is the definition of a set S_ξ for each discrete mode ξ containing the indices of all possible predecessor modes of ξ. For the scenario tree depicted in Figure 3, the mode $\xi=5$ can, for instance, be reached by the modes $\xi=1$ and $\xi=2$ such that the set of predecessors is determined to $S_5=\{1,2\}$. Furthermore, the variables σ_ξ will be used as index variables over the sets S_ξ. The transition to a discrete mode ξ is now possible during a certain time period T_{σ_ξ} in which the system resides in one of the predecessor modes $\sigma_\xi \in S_\xi$. For the mode $\xi=5$ in Figure 3, this convention results in the possible transition times $t^*_{1,5} \in T_1$ and $t^*_{2,5} \in T_2$. If we focus on the time period T_1 for the moment, it can be concluded that this interval ranges from the time $t^*_{0,1}$ where the system switches from $\xi=0$ to $\xi=1$ up to the final time $t_{1,f}$ of $\xi=1$. This holds similarly for the time horizon T_2. The definition of the switching time to one particular mode is therefore based on the switching times to all modes lying on the next upper layer of the discrete structure. This holds recursively up to the root of the scenario tree with $T_0=[t_{0,0}, t_{0,f}]$. As before, specific process models f_ξ and mapping functions $h_{\sigma_\xi,\xi}$ have to be used for each discrete mode such that the resulting mathematical model formulation can be stated as

$$\begin{aligned}
0 &= f_\xi\left(\dot{x}_\xi, x_\xi, y_\xi, u_\xi, t_\xi\right),\\
0 &= h_{\sigma_\xi,\xi}\left(x_{\sigma_\xi}, u_{\sigma_\xi}, x_\xi, u_\xi, t^*_{\sigma_\xi,\xi}\right),\\
&\quad \forall t_\xi \in T_\xi = \left[t^*_{\sigma_\xi,\xi}, t_{\xi,f}\right],\\
&\quad \forall t^*_{\sigma_\xi,\xi} \in T_{\sigma_\xi},\\
&\quad \forall \sigma_\xi \in S_\xi,\\
&\quad \xi = 0, 1, \ldots, N.
\end{aligned} \tag{SIM3}$$

Since the nominal mode does not have any predecessor, the set S_0 is empty and time periods T_{σ_0} do not exist in the conventional sense. In order to keep the notation uniform for all modes, T_{σ_0} is defined as containing the initial time of the nominal mode $t_{0,0}$ only. In addition, the mapping function $h_{\sigma_0,0}$ reduces to the specification of the initial conditions $x_{0,0}$ for the nominal mode. Note that in the notation used, the subscripts for t^* and h indicate two discrete modes, whereas

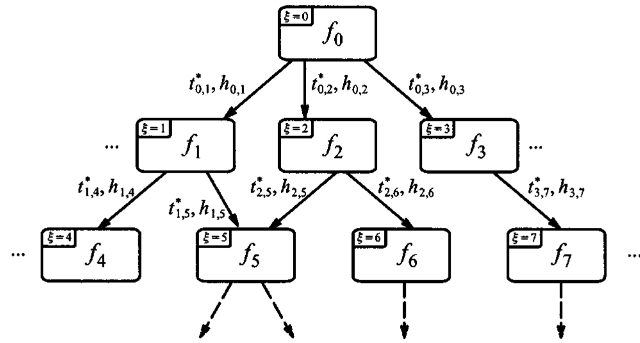

Figure 3. Structure of a scenario-integrated system with multiple transitions.

the indices for all other doubly subscripted variables, such as $t_{\xi,f}$, describe the corresponding discrete mode (first subscript) and a particular instant (second subscript), respectively.

The complexity of the model formulation Model SIM3 is enormous. From the nominal mode, each scenario belonging to a mode on the second layer of Figure 3 can start at any moment during the period T_0. From each of the scenario modes on the second layer the system is then able to switch to a mode on the third layer at any instant of the corresponding scenario horizon T_ξ. This continues until the last level of scenario modes is reached.

Scenario-Integrated Optimization

Having developed model formulations for dynamic systems with incorporated scenarios, we can now start to consider their dynamic optimization. Unfortunately, the theory of hybrid discrete-continuous systems here does not provide an equally sound basis as for modeling and simulation. Rather the dynamic optimization of hybrid systems still seems to be an unsolved problem. The main difficulty is that the number and type of transitions can change during the search for a set of optimal control profiles. In general, this renders the objective function discontinuous with respect to the degrees of freedom, which results in a series of problems. Gradient-based search algorithms are definitely confounded in this case and other approaches have to be applied; see Galan et al. (1998), for an example. Branicky et al. (1998) probably present the most general approach to the optimal control of hybrid systems by extending the quasi-variational inequalities encountered in impulse control (Bensoussan and Lions, 1984), but the assumptions that have to be fulfilled in order to apply their results are difficult to verify for many realistic problems. Galán and Barton (1998) have developed a method for the optimization of hybrid systems that is applicable to cases where the sequence of events does not change during the search process. Obertopp et al. (1998) extend these results to systems that allow several transitions to occur simultaneously. A game-theoretic approach to the synthesis of optimal control strategies for hybrid systems is discussed by Lygeros et al. (1996). These authors, however, restrict the discrete part of the system to the definition of setpoints that change from time to time. An underlying continuous controller is then designed using optimal control theory. Dimitriadis et al. (1996, 1997, 1998) have studied the optimization of hybrid systems with the emphasis on the design of safe process systems. A nonlinear mixed-integer dynamic optimization problem is formulated in order to drive the process into the most unsafe part of the state space. As long as this remains impossible, the system can be called safe.

For the purposes of this article, these attempts are inapplicable, since the uncertainty in the switching time cannot be captured properly. New approaches must therefore be developed. The resulting dynamic optimization problems can be divided into two subclasses introduced earlier. In *single-level scenario-integrated optimization problems,* the nature of the scenario modes and the operational goals favor the use of the same economic objective function independently of any event that may occur during the transient phase of the process. In contrast, *bilevel scenario-integrated optimization problems* aim at an economic optimization in the nominal mode, with only secondary goals defined for the scenario modes.

Single-level scenario-integrated optimization

The formulation of scenario-integrated dynamic optimization problems is quite complex. In order to provide an easy access to these problems the discussion will proceed stepwise, starting with only one scenario mode. First, it will be assumed that the switching time of the possible transition is known. The results will then be generalized to the case of an unknown switching time before briefly discussing optimization problems for multiple scenarios.

Single Scenario With Fixed Transition Time. If the number of possible scenario modes is limited to one, and if the switching time is assumed to be known, the existing uncertainty is reduced to the question of whether or not the event triggering the scenario will occur. This situation is illustrated in Figure 4, which shows the evolution of one state and one manipulated variable. The system evolves in the nominal mode along the trajectories of $u_0(t_0)$ and $x_0(t_0)$ up to the switching time $t^*_{0,1}$. Then it may switch to the scenario mode, resulting in the trajectories $u_1(t_1)$ and $x_1(t_1)$ or rest in the nominal mode $\xi = 0$. The optimization problem is to find profiles of the available operational degrees of freedom $u_0(t_0)$ and $u_1(t_1)$, which minimize the chosen objective function under the set of given constraints.

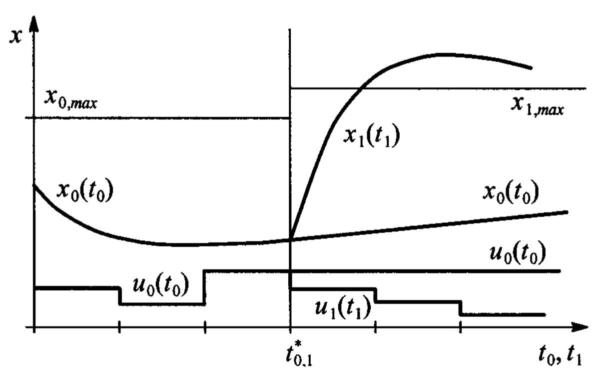

Figure 4. Evolution of a state and a manipulated variable within the nominal and the scenario mode.

The first problem to discuss is the choice of an appropriate objective function. If the approach taken in stochastic programming for parametric uncertainties is adopted, probabilities have to be associated with the two possible cases, and a weighted objective function

$$\Phi = w_0\Phi_0\left(x_0, u_0, t_{0,f}\right) + w_1\Phi_1\left(x_1, u_1, t_{1,f}\right), \qquad (9)$$

with $\mathbf{\Phi}_0 : \mathbb{R}^{n_0}\times\mathbb{R}^{m_0}\times\mathbb{R}^{p_0}\times\mathbb{R}\to\mathbb{R}$ and $\mathbf{\Phi}_1 : \mathbb{R}^{n_1}\times\mathbb{R}^{m_1}\times\mathbb{R}^{p_1}\times\mathbb{R}\to\mathbb{R}$, must be minimized. The weights w_0 and w_1 correspond to the probability that the system resides in $\xi = 0$ and $\xi = 1$ after $t^*_{0,1}$, with $w_0 + w_1 = 1$. It is interesting to note that a second interpretation of the objective function in Eq. 9 exists. This interpretation originates in the theory of multicriteria optimization (Clark and Westerberg, 1983; Hwang et al., 1980; Tsoukas et al., 1982), where several objective functions are supposed to be minimized simultaneously. For the system shown in Figure 4, one objective function would be formulated for the case where a transition occurs at $t^*_{0,1}$ and another one for the case where it does not occur. Typically, one of these objective functions cannot be reduced without increasing at least one of the others. The solution of these problems is no longer unique, but forms a set of Pareto-optimal or effective values. One technique commonly applied to obtain a unique solution of multicriteria optimization problems is to assume a decision-maker defining weighting factors for each of the objective functions. This transforms the vector-valued objective function into a scalar one of the type embodied in Eq. 9.

According to the results previously obtained, the process models for the nominal and the scenario modes generally differ. It is therefore consistent, and for many cases also desirable, to allow scenario-specific constraints. If these constraints are denoted by $g_0 : \mathbb{R}^{n_0}\times\mathbb{R}^{m_0}\times\mathbb{R}^{p_0}\times\mathbb{R}\to\mathbb{R}^{c_0}$ and $g_1 : \mathbb{R}^{n_1}\times\mathbb{R}^{m_1}\times\mathbb{R}^{p_1}\times\mathbb{R}\to\mathbb{R}^{c_1}$, where c_0 and c_1 are the number of constraints in the nominal and the scenario modes, the simplest scenario-integrated dynamic optimization problem can be formulated as

$$\begin{aligned}
\min_{\substack{x_{0,0},\, u_0(t_0),\, t_{0,f},\\ u_1(t_1),\, t_{1,f}}} \quad & w_0\Phi_0\left(x_0, y_0, u_0, t_{0,f}\right) + w_1\Phi_1\left(x_1, y_1, u_1, t_{1,f}\right) \\
\text{s.t.} \quad & 0 = f_0\left(\dot{x}_0, x_0, y_0, u_0, t_0\right), \\
& 0 = x_0\left(t_{0,0}\right) - x_{0,0}, \\
& 0 \ge g_0\left(x_0, y_0, u_0, t_0\right), \qquad \text{(SIOP1)} \\
& \quad \forall t_0 \in \left[t_{0,0}, t_{0,f}\right], \\
& 0 = f_1\left(\dot{x}_1, x_1, y_1, u_1, t_1\right), \\
& 0 = h_{0,1}\left(x_0, u_0, x_1, u_1, t^*_{0,1}\right), \\
& 0 \ge g_1\left(x_1, y_1, u_1, t_1\right), \\
& \quad \forall t_1 \in \left[t^*_{0,1}, t_{1,f}\right].
\end{aligned}$$

The initial conditions for the nominal mode $x_{0,0}$ and for the final times $t_{0,f}$ and $t_{1,f}$ have been regarded as degrees of freedom. If these variables are fixed for specific problems, appropriate equations might be formulated as additional constraints.

Single Scenario with Unknown Transition Time. Assuming that there is a known transition time to the scenario mode is, of course, unjustified for most realistic problems. The question therefore is how Problem SIOP1 can be extended to cope with the uncertainty in the switching time. Because of the infinite number of possible transition times, this extension complicates the problem considerably. In order to find a way of incorporating the complete set of possible scenarios into the dynamic optimization problem, we will again use an approach that originated in the field of stochastic programming. There, the infinite number of parameter values is tackled by multiplying the objective function by the probability density function of the uncertain parameter and integrating over the uncertainty domain. This approach can also be applied to the uncertain transition time. This results in the problem structure

$$\min \int_{-\infty}^{\infty} p(t_{0,1}^{*})\Phi(t_{0,1}^{*})\,dt_{0,1}^{*}. \tag{10}$$

It has already been argued that the statistical data for determining a detailed probability density function $p(t_{0,1}^{*})$ are often not available. In the absence of further knowledge, it can only be assumed that the probability of the system switching to the scenario mode is constant for all instants $t_{0,1}^{*} \in [t_{0,0}, t_{0,f}]$. Thus, the probability density function for the uncertain transition time can be stated as

$$p(t_{0,1}^{*}) = w_0\,\delta\left(t_{0,1}^{*} - \hat{t}\right) + w_1\left[\sigma\left(t_{0,1}^{*} - t_{0,0}\right) - \sigma\left(t_{0,1}^{*} - t_{0,f}\right)\right], \tag{11}$$

with w_0 and w_1 chosen such that the integral of $p(t_{0,1}^{*})$ over the domain of uncertainty gives unity. Here, δ denotes the Dirac impulse and σ the step function. The time $\hat{t} \notin [t_{0,0}, t_{0,f}]$ has been introduced for formal reasons only and is associated with the nominal operation. Inserting Eq. 11 into Eq. 10 and rearranging the integrand results in the scenario-integrated dynamic optimization problem for a single scenario mode and an unknown switching time:

$$\begin{aligned}
\min_{\substack{x_{0,0},\, u_0(t_0),\, t_{0,f},\\ u_1(t_1),\, t_{1,f}}} \quad & w_0\Phi_0\left(x_0, y_0, u_0, t_{0,f}\right) \\
& + w_1\int_{t_{0,0}}^{t_{0,f}} \Phi_1\left(x_1, y_1, u_1, t_{1,f}\right) dt_{0,1}^{*} \\
\text{s.t.}\quad & 0 = f_0(\dot{x}_0, x_0, y_0, u_0, t_0), \\
& 0 = x_0(t_{0,0}) - x_{0,0}, \\
& 0 \geq g_0(x_0, y_0, u_0, t_0), \\
& \qquad \forall t_0 \in \left[t_{0,0}, t_{0,f}\right], \\
& 0 = f_1(\dot{x}_1, x_1, y_1, u_1, t_1), \\
& 0 = h_{0,1}(x_0, u_0, x_1, u_1, t_{0,1}^{*}), \\
& 0 \geq g_1(x_1, y_1, u_1, t_1), \\
& \qquad \forall t_1 \in \left[t_{0,1}^{*}, t_{1,f}\right], \\
& \qquad \forall t_{0,1}^{*} \in \left[t_{0,0}, t_{0,f}\right].
\end{aligned} \tag{SIOP2}$$

Recall from the discussion of the scenario-integrated model that the trajectories of the manipulated variables and the final times in the scenario mode depend on the switching time $t_{0,1}^{*}$, which is not explicitly shown in the notation used here. The consequence, however, is that the solution of Problem SIOP2 yields a single trajectory for the variables $u_0(t_0)$, an infinite number of trajectories for $u_1(t_1)$ in the t_0-t_1-u_1 space, and an infinite number of final times $t_{1,f}$. This is the main difference from stochastic optimization approaches that look for one single trajectory reflecting all possible switching times. Furthermore, the dynamic optimization Problem SIOP2 is subject to the model descriptions and the constraints of the nominal and the scenario modes.

It should be noted that Problem SIOP2 could also be derived from the multicriteria perspective. In that case, factors w_0 and w_1 would be chosen as independent weighting factors. Through normalization, it can always be achieved that the optimization problem obtained from the multicriteria perspective differs from Problem SIOP2 only by a constant factor that does not change the calculated optimal solution.

Multiple Scenarios and Scenario Trees. The generalization of these results to multiple scenarios is straightforward as long as only one single layer of scenario modes exists below the nominal mode in the structure of Figure 3. Since the various scenario modes are completely decoupled, the joint probability density function to be applied in the formulation of the objective function can be stated as

$$\begin{aligned}
p(t_{0,1}^{*}, t_{0,2}^{*}, \ldots, t_{0,N}^{*}) = {} & w_0\,\delta\left(t_{0,1}^{*} - \hat{t}\right) \\
& + w_1\left[\sigma\left(t_{0,1}^{*} - t_{0,0}\right) - \sigma\left(t_{0,1}^{*} - t_{0,f}\right)\right] \\
& \vdots \\
& + w_N\left[\sigma\left(t_{0,N}^{*} - t_{0,0}\right) - \sigma\left(t_{0,N}^{*} - t_{0,f}\right)\right],
\end{aligned}$$

The corresponding scenario-integrated dynamic optimization problem can therefore be formulated directly from Problem SIOP2:

$$\begin{aligned}
\min_{\substack{x_{0,0},\, u_0(t_0),\, t_{0,f},\\ u_1(t_1),\, t_{1,f},\, \ldots,\, u_N(t_N),\, t_{N,f}}} \quad & w_0\Phi_0\left(x_0, y_0, u_0, t_{0,f}\right) \\
& + \sum_{\xi=1}^{N} w_\xi \int_{t_{0,0}}^{t_{0,f}} \Phi_\xi\left(x_\xi, y_\xi, u_\xi, t_{\xi,f}\right) dt_{0,\xi}^{*}.
\end{aligned} \tag{SIOP3}$$

Problem SIOP3 is subject to Model SIM2 as well as the constraints g_0 and g_ξ. An infinite number of trajectories of the manipulated variables has again to be determined, this time for all N scenario modes under consideration.

It is much more difficult to develop optimization problems for the complete scenario tree shown in Figure 3, since the combinatorial nature of these problems adds an additional level of complexity. In principle, an appropriate objective function must be combined with the model formulation SIM3 and the existing constraints for all discrete modes involved. In contrast to the optimization problems formulated so far, it seems to be impossible to use available numerical techniques to calculate solutions for problems involving scenario trees, at least for the moment. For the purposes of this article, we will therefore restrict ourselves to the scenario-integrated dynamic optimization problems SIOP3, leaving more general problems for further research.

Bilevel scenario-integrated optimization

The second possibility for optimizing a dynamic system with integrated scenarios is to formulate a bilevel optimization problem. Again starting with a single scenario and a known switching time, we formulate such a problem in the following subsection before generalizing the results to multiple scenarios. Two interesting special cases are presented at the end of this section.

Single Scenario. A convenient starting point for the development of bilevel scenario-integrated dynamic optimization problems is again the situation depicted in Figure 4, where a fixed transition time was treated and the only uncertainty is if the system switches to the scenario mode at $t^*_{0,1}$. Throughout the subsection on single-level scenario-integrated optimization it was assumed that these two cases are in principle of equal importance. If an optimization of the system behavior in the nominal mode is of preferred interest, however, the treatment of the scenario mode has to focus only on the enforcement of existing constraints. In Figure 4 these constraints compose an upper limit on the state variable for the nominal and the scenario modes, $x_{0,\max}$ and $x_{1,\max}$. Obviously, the latter is violated. Two possibilities now exist to enforce the constraint. First, the manipulated variable of the scenario mode $u_1(t_1)$ can be changed. Second, the initial condition of the scenario mode $x_1(t^*_{0,1})$, which is determined by the mapping function $0 = h_{0,1} = x_0(t^*_{0,1}) - x_1(t^*_{0,1})$, can be changed such that a violation can no longer be observed. This can be achieved indirectly by manipulating the variable $u_0(t_0)$ or the initial condition $x_{0,0}$ of the nominal mode. When there is a higher economic priority of the nominal mode, the preferred choice between these two possibilities will always lie on $u_1(t_1)$ so that $u_0(t_0)$ and $x_{0,0}$ can be reserved in order to achieve the best possible performance. If this is sufficient for all possible scenarios, the two dynamic optimization problems can be decoupled. The scenario optimization problem is then solved after the optimum of the nominal optimization problem has been determined. Due to the infinite number of switching times $t^*_{0,1}$, an infinite number of scenario optimization problems has to be solved in this case. If, however, input constraints or a low sensitivity of the constrained variable with respect to the manipulated variable prevent the enforcement of the scenario constraints with $u_1(t_1)$ only, the operation in the nominal mode must also be adjusted appropriately. The optimization problem in the scenario mode then behaves as an implicit constraint to the optimization of the nominal mode.

Stationary problems of this kind can be found in the area of bilevel programming (Cheng and Florian, 1995; Falk and Liu, 1995). In chemical engineering, Clark and Westerberg (1983, 1990a,b) have studied bilevel programming problems extensively in the context of an optimal steady-state design of equilibrium processes. The number and nature of the existing thermodynamic phases were assumed to be unknown, necessitating the minimization of the Gibbs free energy as a subtask of the original optimal design problem. An extension to a dynamic subproblem was presented by Brengel and Seider (1992). Their goal was to find the optimal operating conditions of chemical processes equipped with model predictive controllers. These controllers must enforce a number of constraints, and their ability to achieve this depends on the chosen operating point determined by the master problem.

For the scenario-integrated optimization problem discussed here, the main problem in the nominal mode and the subproblem in the scenario mode are *both* dynamic optimization problems, and hence generalize the problems of Clark and Westerberg (1990a) and Brengel and Seider (1992). For a fixed switching time, the resulting formulation can be mathematically stated as:

$$
\begin{aligned}
&\min_{x_{0,0},\, u_0(t_0),\, t_{0,f}} \Phi_0(x_0, y_0, u_0, t_{0,f})\\
&\text{s.t. } 0 = f_0(\dot{x}_0, x_0, y_0, u_0, t_0),\\
&\quad 0 = x_0(t_{0,0} - x_{0,0}),\\
&\quad 0 \geq g_0(x_0, y_0, u_0, t_0),\\
&\quad\quad \forall t_0 \in [t_{0,0}, t_{0,f}],\\
&\qquad\qquad \min_{u_1(t_1),\, t_{1,f}} \Psi_1(x_1, y_1, u_1, t_{1,f})\\
&\text{s.t. } 0 = f_1(\dot{x}_1, x_1, y_1, u_1, t_1),\\
&\quad 0 = h_{0,1}(x_0, u_0, x_1, u_1, t^*_{0,1}),\\
&\quad 0 \geq g_1(x_1, y_1, u_1, t_1),\\
&\quad\quad \forall t_1 \in [t^*_{0,1}, t_{1,f}],
\end{aligned}
\tag{SIOP4}
$$

with a specific objective function $\Psi_1 : \mathbb{R}^{n_1} \times \mathbb{R}^{m_1} \times \mathbb{R}^{p_1} \times \mathbb{R} \rightarrow \mathbb{R}$ for the scenario mode. Since the mapping function $h_{0,1}$ determines variables of the subproblem in SIOP4 on the basis of information obtained in the nominal mode, the master and the subproblem are coupled. In contrast to other bilevel optimization problems, however, there is no coupling from the subproblem back to the master problem.

The generalization of Problem SIOP4 to the realistic case of an unknown switching time $t^*_{0,1}$ follows the same line as used for the single-level optimization problems. An infinite number of possible initial conditions for the scenario optimization problem now have to be treated. Consequently, the subproblem in SIOP4 must now be formulated for all $t^*_{0,1} \in [\mathrm{t}_{0,0}, t_{0,f}]$, which results in an infinite number of dynamic optimization problems restricting the master optimal control problem in the nominal mode. The derivation of the corresponding mathematical formulation is relatively straightforward and is omitted here since it turns out to be a special case of the multiple-scenario situation discussed next.

Multiple Scenarios. If the treatment of bilevel optimization problems with multiple scenarios is again limited to one single layer of possible scenario modes, the system is able to switch to all these modes at any moment within the time horizon of the nominal mode $[t_{0,0}, t_{0,f}]$. The mathematical problem formulation for this case can be derived by directly extending Problem SIOP4:

$$
\begin{aligned}
&\min_{x_{0,0},\, u_0(t_0),\, t_{0,f}} \quad \Phi_0(x_0, y_0, u_0, t_{0,f}) \\
&\text{s.t.}\;\; 0 = f_0(\dot{x}_0, x_0, y_0, u_0, t_0), \\
&\quad 0 = x_0(t_{0,0}) - x_{0,0}, \\
&\quad 0 \ge g_0(x_0, y_0, u_0, t_0), \\
&\qquad \forall t_0 \in [t_{0,0}, t_{0,f}], \qquad\qquad \text{(SIOP5)} \\
&\qquad \min_{u_\xi(t_\xi),\, t_{\xi,f}} \quad \Psi_\xi(x_\xi, y_\xi, u_\xi, t_{\xi,f}) \\
&\text{s.t.}\;\; 0 = f_\xi(\dot{x}_\xi, x_\xi, y_\xi, u_\xi, t_\xi), \\
&\quad 0 = h_{0,\xi}(x_0, u_0, x_\xi, u_\xi, t^*_{0,\xi}), \\
&\quad 0 \ge g_\xi(x_\xi, y_\xi, u_\xi, t_\xi), \\
&\qquad \forall t_\xi \in [t^*_{0,\xi}, t_{\xi,f}], \\
&\qquad \forall t^*_{0,\xi} \in [t_{0,0}, t_{0,f}], \\
&\qquad \xi = 1, \ldots, N,
\end{aligned}
$$

where an infinite number of subproblems is formulated for each of the N scenario modes under consideration.

Significantly more difficult is the development of problem formulations with more than one layer of scenario modes. One probably would have to distinguish between cases that require a third or even more layers of optimization problems and cases where the formulation of objective functions can be restricted to the bilevel type. These problems are not only of theoretical but also of practical interest, since the question of how subsequent multiple failures can be tackled as part of the dynamic optimization problems would lead to such a structure. Finding an answer to this question is, however, beyond the scope of this article, and requires additional research effort.

Special Cases. On the basis of the bilevel dynamic optimization Problem SIOP5, two interesting special cases can be derived. The first case arises if a stationary process is considered in the nominal mode. The degrees of freedom u_0 then comprise time-invariant variables only. Furthermore, the process model f_0 for the nominal mode now consists of a set of algebraic equations, yielding an inherent structural difference between f_0 and the dynamic model equations f_ξ valid in the scenario modes. Nevertheless, note that Problem SIOP5 does not reduce to a conventional dynamic optimization problem and that the bilevel structure is still preserved. The determination of an optimal operating point for a process under predictive model control (Brengel and Sieder, 1992) mentioned earlier belongs to this problem class. A second example is the determination of optimal operating points for stationary processes together with rapid shutdown policies to be applied under externally triggered conditions.

The second special case comprises scenario modes that do not provide any operational degree of freedom. As can be concluded from Examples 5 and 6, this situation is very realistic. Such problems will never be formulated as single-level problems where an economic optimization is also carried out in the scenario mode. Clearly, they show a bilevel character with an emphasis in the scenario mode on enforcing the existing constraints. In contrast to Problem SIOP5, however, the formulation of an objective function Ψ_ξ is not meaningful without access to some associated degrees of freedom. The bilevel dynamic optimization problem therefore reduces to

$$
\begin{aligned}
&\min_{x_{0,0},\, u_0(t_0),\, t_{0,f}} \quad \Phi_0(x_0, y_0, u_0, t_{0,f}) \\
&\text{s.t.}\;\; 0 = f_0(\dot{x}_0, x_0, y_0, u_0, t_0), \\
&\quad 0 = x_0(t_{0,0}) - x_{0,0}, \\
&\quad 0 \ge g_0(x_0, y_0, u_0, t_0), \\
&\qquad \forall t_0 \in [t_{0,0}, t_{0,f}], \qquad\qquad \text{(SIOP6)} \\
&\quad 0 = f_\xi(\dot{x}_\xi, x_\xi, y_\xi, t_\xi), \\
&\quad 0 = h_{0,\xi}(x_0, u_0, x_\xi, t^*_{0,\xi}), \\
&\quad 0 \ge g_\xi(x_\xi, y_\xi, t_\xi), \\
&\qquad \forall t_\xi \in [t^*_{0,\xi}, t_{\xi,f}], \\
&\qquad \forall t^*_{0,\xi} \in [t_{0,0}, t_{0,f}], \\
&\qquad \xi = 1, \ldots, N.
\end{aligned}
$$

To the authors' knowledge these problems were treated in Abel et al. (1998) for the first time. Although they no longer show a tiered optimization structure, they have still to be analyzed along multiple time axes with an infinite number of initial conditions on the time axis of the scenario modes.

Numerical Solution Approach

So far, the emphasis in this article has been on the development of an appropriate model framework for scenario-integrated dynamic systems and on the derivation of appropriate formulations for their optimization. The question of how these problems can be solved for practical problems has not yet been treated. This section therefore focuses on this point.

From the previous discussion it can be concluded that the complexity of scenario-integrated optimization problems rarely allows an analytical solution. Thus, numerical solution techniques have to be applied. For hybrid systems and stochastic problems such techniques are still subject to active research. Robust and efficient algorithms are often not available. Even worse is the situation in bilevel programming where numerical techniques face severe difficulties. For example, it is known that bilevel programming problems can be nonconvex even if the objective functions and the feasible sets of the master problem and the subproblem are convex (Clark and Westerberg, 1990a). At present, it is therefore only possible to tackle scenario-integrated dynamic optimization problems by solving simplified problems that approximate the formulations derived earlier. Since approximation is inherent in any numerical solution technique, this must not be seen as a major drawback as long as the characteristic features are preserved. In this sense, the following subsections present a first attempt at solving the single- and bilevel scenario-integrated optimization Problems SIOP3 and SIOP6.

Reducing the problem dimensionality

With respect to the numerical solution the main problem of all formulations derived is given by the unknown switching times $t^*_{0,\xi}$ to the scenario modes. This requires the consideration of an infinite number of possible switching times. A similar problem arises in stochastic programming where an infinite number of possible parameter values have to be treated, and the objective function usually contains an integral expression over the original cost function multiplied by the probability density function. The common approach to solving these problems is to replace the integral by a finite sum employing an appropriate sampling strategy (Birge and Louveaux, 1997). This technique is also applied here for the solution of scenario-integrated optimization problems.

The single-level dynamic optimization Problem SIOP3 integrating N scenario modes can then be approximated by

$$\begin{aligned}
\min_{\substack{x_{0,0},\, u_0(t_0),\, t_{0,f},\\ u_1(t_{1,k}),\, t_{1,f,k},.,\, u_N(t_{N,k}),\, t_{N,f,k}}} \quad & w_0 \Phi_0(x_0, y_0, u_0, t_{0,f}) \\
& + \sum_{\xi=1}^{N} w_\xi \sum_{k=1}^{K} \Phi_{\xi,k}(x_{\xi,k}, y_{\xi,k}, u_{\xi,k}, t_{\xi,f,k}) \\
\text{s.t.} \quad & 0 = f_0(\dot{x}_0, x_0, y_0, u_0, t_0), \\
& 0 = x_0(t_{0,0}) - x_{0,0}, \\
& 0 \geq g_0(x_0, y_0, u_0, t_0), \\
& \forall t_0 \in [t_{0,0}, t_{0,f}], \qquad\qquad \text{(SIOPA)} \\
& 0 = f_{\xi,k}(\dot{x}_{\xi,k}, x_{\xi,k}, y_{\xi,k}, u_{\xi,k}, t_{\xi,k}), \\
& 0 = h_{0,\xi,k}(x_0, u_0, x_{\xi,k}, u_{\xi,k}, t^*_{0,\xi,k}), \\
& 0 \geq g_{\xi,k}(x_{\xi,k}, y_{\xi,k}, u_{\xi,k}, t_{\xi,k}), \\
& \forall t_{\xi,k} \in [t^*_{0,\xi,k}, t_{\xi,f,k}], \\
& t^*_{0,\xi,k} = t_{0,k}, \\
& k = 1, \ldots, K, \\
& \xi = 1, \ldots, N.
\end{aligned}$$

Here, K instants $t_{0,k} \in [t_{0,0}, t_{0,f}]$ have been chosen on the time axis of the nominal mode. Only at these instants are transitions to the scenario modes possible. Consequently, the analysis of the system under consideration is no longer performed on a complete surface, but only along a finite number of trajectories in the space spanned by the time axes and the state variables. This was already indicated in Figure 2 by the lines evolving on the gray surface along the t_1-axis.

The same approach of defining finitely many instants $t_{0,k}$ on the time axis of the nominal mode can also be used in order to derive an approximation for Problem SIOP6. This results in an optimal control problem minimizing Φ_0 only and manipulating the degrees of freedom in the nominal mode $x_{0,0}$, $u_0(t_0)$, and $t_{0,f}$. The problem is subject to the same constraints as stated in Problem SIOPA, with the one difference that the degrees of freedom $u_{\xi,k}$ do not exist.

It should be noted that an analogous simplification has already been used for the treatment of state variable inequality constraints in conventional dynamic optimization problems. For path constraints, the requirement for their exact satisfaction at all instants within $[t_0, t_f]$ has been replaced by testing their values at a restricted number of interior points; see, for instance, Vassiliades et al. (1994b). These points are usually chosen sufficiently close together to prevent severe constraint violations in between. For the solution of conventional dynamic optimization problems, however, alternative methods for the enforcement of inequality path constraints on state variables do also exist. One of these methods is the definition of an additional state variable integrating the constraint violation over time. This variable is then forced to zero at the final time by an appropriate endpoint constraint. Feehery and Barton (1998) recently presented another approach, which adds an equation to the process model as soon as an inequality constraint becomes active. However, both techniques cannot be directly applied to scenario-integrated optimization problems, since they require explicit function evaluations. Thus, the (less rigorous) technique chosen currently seems to be the only feasible solution approach.

Control vector parameterization

Problem SIOPA almost has the structure of a conventional dynamic optimization problem. Several established numerical techniques for solving these problems exist. In general, direct and indirect methods can be recognized (Von Stryk and Bulirsch, 1992). Indirect methods formulate the necessary optimality conditions which lead to a multipoint boundary-value problem. Even for conventional dynamic systems this problem can be difficult to solve, since unstable modes have to be integrated either in the forward or in the backward direction. The incorporation of discontinuities into these methods is not trivial, although some results are available for the simple case where the model structure does not change and the instant of the discontinuity is known *a priori* (Bryson and Ho, 1975).

Direct approaches convert the dynamic optimization problem to a nonlinear programming problem (NLP) through the parameterization of the state and the manipulated variables (Cuthrell and Biegler, 1987) or through the parameterization of the manipulated variables only (Vassiliadis et al., 1994a,b). The latter technique is also called control vector parameterization, since the profiles of the operational degrees of freedom $u(t)$ are described by

$$u(t) = \sum_{j=1}^{M} \vartheta_j \varphi_j(t), \tag{12}$$

where $\varphi_j(t)$ comprise appropriate local or global basis functions. Often, piecewise-linear or piecewise-constant parameterizations are chosen along the various time axes. The variables ϑ_j are time-invariant parameters. They are collected in the parameter vector $\boldsymbol{\theta}$ together with other free optimization parameters. For a specific choice of $\boldsymbol{\theta}$, the $N * K + 1$ initial-value problems in Problem SIOPA are first solved by state-of-the-art DAE integrators. The result is then passed to an NLP solver that generates improved values for $\boldsymbol{\theta}$. If gradient-based algorithms are used for the solution of the NLP, it is necessary to determine the sensitivities of the objective function and the constraints with respect to the free optimization variables $\boldsymbol{\theta}$. This can be achieved simultaneously with the integration of the DAE system. The sequential execution of integration and optimization continues until some specified convergence criteria are met.

Currently, this approach seems to be the most promising for the treatment of systems containing continuous and discrete dynamics (Allgor and Barton, 1997; Barton et al., 1998) since the switching functions l_{ξ_i,ξ_j} can be formulated as additional model equations, and their sign changes corresponding to the discrete events can be properly detected during the integration of the DAEs. Equation 12 must then be stated for all discrete modes $\xi = 0, 1, \ldots, N$, and a parameter vector $\boldsymbol{\theta}_\xi$ can be associated with each of these modes.

Calculation of sensitivities

In principle, both the objective function and the constraints can be formulated as (additional) model equations. Therefore, the calculation of sensitivities can be restricted here to the sensitivities of f_ξ, with $\xi = 0, \ldots, N$. Differentiating these equations with respect to the free optimization parameters $\boldsymbol{\theta}_\xi$ results in

$$0 = \frac{\partial f_\xi}{\partial \dot{x}_\xi}\dot{s}_{x,\xi} + \frac{\partial f_\xi}{\partial x_\xi}s_{x,\xi} + \frac{\partial f_\xi}{\partial y_\xi}s_{y,\xi} + \frac{\partial f_\xi}{\partial \boldsymbol{\theta}_\xi}, \tag{13}$$

with the sensitivity variables

$$s_{x,\xi} = \frac{\partial x_\xi}{\partial \boldsymbol{\theta}_\xi}, \qquad s_{y,\xi} = \frac{\partial y_\xi}{\partial \boldsymbol{\theta}_\xi}. \tag{14}$$

Equation 13 can be integrated simultaneously with the model equations, exploiting the same Jacobian matrices as used for the model equations (Caracotsios and Stewart, 1985; Feehery et al., 1997; Maly and Petzold, 1996).

Of particular importance is the behavior of $s_{x,\xi}$ and $s_{y,\xi}$ at the switching times $t^*_{0,\xi}$. It is known that both variables will generally jump at these points (Bryson and Ho, 1975; Rosen and Luus, 1991), and particular attention must be paid in order to calculate the gradient information correctly. With respect to the behavior of the sensitivities at the transitions, Galán and Barton (1998) classify the optimization of hybrid systems as follows:

1. The sequence of discrete modes does not always remain the same between subsequent iterations of the search process in the NLP.
2. The sequence of discrete modes remains unchanged during the search process, but the sensitivity variables jump at the switches.
3. The sequence of discrete modes remains unchanged during the search process and the sensitivity variables do not jump at the switches.

Only two specific layers of discrete modes exist for the Problems SIOP3 and SIOP6, and the systems always switch from the nominal mode to the scenario mode. Therefore, the sequence of discrete modes remains unchanged and the problems treated here do not belong to the first class. In order to determine whether the sensitivity variables $s_{x,\xi}$ and $s_{y,\xi}$ jump at the transitions, the total derivatives of $l_{0,\xi}$ and $h_{0,\xi}$ have to be examined at the switching times $t^*_{0,\epsilon}$ (Obertopp et al., 1998). Specifying $\xi_i = 0$ and $\xi_j = \xi$ in Eq. 7, stating $l_{0,\xi} = t_0 - t^*_{0,\xi}$, and employing the parameterization of Eq. 12, these expressions are calculated as

$$\frac{dl_{0,\xi}}{d\boldsymbol{\theta}_0} = \frac{\partial l_{0,\xi}}{\partial t_0}\frac{dt_0}{d\boldsymbol{\theta}_0} + \frac{dl_{0,\xi}}{dt^*_{0,\xi}}\frac{dt^*_{0,\xi}}{d\boldsymbol{\theta}_0} = 0, \tag{15}$$

$$\frac{dh_{0,\xi}}{d\boldsymbol{\theta}_0} = \frac{\partial h_{0,\xi}}{\partial x_0}\frac{dx_0}{d\boldsymbol{\theta}_0} + \frac{\partial h_{0,\xi}}{\partial \boldsymbol{\theta}_0} + \frac{\partial h_{0,\xi}}{\partial x_\xi}\frac{dx_\xi}{d\boldsymbol{\theta}_0} + \frac{\partial h_{0,\xi}}{\partial \boldsymbol{\theta}_\xi} + \frac{\partial h_{0,\xi}}{\partial t^*_{0,\xi}}\frac{dt^*_{0,\xi}}{d\boldsymbol{\theta}_0} = 0, \tag{16}$$

with

$$\frac{dx_0}{d\boldsymbol{\theta}_0} = \frac{\partial x_0}{\partial \boldsymbol{\theta}_0} + \frac{\partial x_0}{\partial t^*_{0,\xi}}\frac{dt^*_{0,\xi}}{d\boldsymbol{\theta}_0}, \tag{17}$$

$$\frac{dx_\xi}{d\boldsymbol{\theta}_0} = \frac{\partial x_\xi}{\partial \boldsymbol{\theta}_0} + \frac{\partial x_\xi}{\partial t^*_{0,\xi}}\frac{dt^*_{0,\xi}}{d\boldsymbol{\theta}_0}. \tag{18}$$

The time t_0 in Eq. 15 does not depend on the optimization variables $\boldsymbol{\theta}_0$, and the first term in this equation therefore vanishes. Since $\partial l_{0,\xi}/\partial t^*_{0,\xi} = -1$, Eq. 15 can only be fulfilled if

$$\frac{dt^*_{0,\xi}}{d\boldsymbol{\theta}_0} = 0. \tag{19}$$

This implies that the switching time $t^*_{0,\xi}$ does not depend on the free variables $\boldsymbol{\theta}_0$, a result that agrees with the earlier discussions. Inserting Eq. 19 into Eqs. 16, 17, and 18 yields

$$\frac{\partial h_{0,\xi}}{d\boldsymbol{\theta}_0} = \frac{\partial h_{0,\xi}}{\partial x_0}\frac{\partial x_0}{\partial \boldsymbol{\theta}_0} + \frac{\partial h_{0,\xi}}{\partial \boldsymbol{\theta}_0} + \frac{\partial h_{0,\xi}}{\partial x_\xi}\frac{\partial x_\xi}{\partial \boldsymbol{\theta}_0} + \frac{\partial h_{0,\xi}}{\partial \boldsymbol{\theta}_\xi} = 0. \tag{20}$$

So far no assumptions have been made on the structure of $h_{0,\xi}$. One specific but frequent case is to assume continuity of the differential variables at the transition

$$h_{0,\xi} = x_0(t^*_{0,\xi}) - x_\xi(t^*_{0,\xi}) = 0. \tag{21}$$

In this case, $h_{0,\xi}$ does not depend explicitly on the parameters $\boldsymbol{\theta}_0$, and Eq. 20 simplifies to

$$\frac{\partial x_0}{\partial \boldsymbol{\theta}_0} - \frac{\partial x_\xi}{\partial \boldsymbol{\theta}_0} = 0. \tag{22}$$

Thus, the sensitivities of the continuous state variables with respect to the free variables will be continuous at transitions of the type expressed by Eq. 21. Whether a particular scenario-integrated system belongs to the second or third class introduced by Galán and Barton (1998) therefore depends on the structure of the transition mapping, and thus on the treated problem. For continuous differential variables at the transitions the existing solution algorithms using control-vector parameterization are directly applicable. In all other cases, a sensitivity correction term has to be calculated at any $t_{0,\xi}^*$ by solving Eq. 20.

Implementation

In our software environment, the model equations f_0 and f_ξ, along with the adjoined sensitivity equations, are integrated using a sparse matrix version (Mangold, 1998) of the code DDASAC (Caracotsios and Stewart, 1985). The nonlinear programs are solved by NPSOL (Gill et al., 1986) employing an SQP strategy (Gill et al., 1981). For free end-time problems the times are scaled by the final times $t_{0,f}$ and $t_{\xi,f,k}$, respectively, which then become additional parameters of the corresponding models [see, for example, Rosen and Luus (1991) for details].

Examples

In order to illustrate the applicability of the derived formulations, two examples of different complexity will be presented. Both are related to failure situations and, for the sake of simplicity, only one scenario is considered ($N = 1$). In the examples treated, only equally spaced, piecewise-constant polynomials are employed as parameterization of the time−varying operational degrees of freedom.

Car problem

The first case study to be treated deals with the car problem that was introduced as Example 5. The distance to be covered in minimum time is 300 m, with the wall placed at 350 m. For nominal operation, the car must start and stop at zero velocity, has a speed limit of 10 m/s, and is subject to limited (normalized) acceleration. The possible brake failure is modeled through a reduction of the maximum available deceleration force to 10% of the nominal value. It is assumed that the driver will always apply this maximum brake force such that the existing time-varying operational degree of freedom is fixed for the scenario mode. The constraints for the system behavior after the brake failure comprise the restriction that the distance of 350 m must never be exceeded and that the car must stop at the endpoint $t_{1,f}$ of the scenario time period.

Because there are no degrees of freedom, the minimization of the final time in the scenario mode does not make

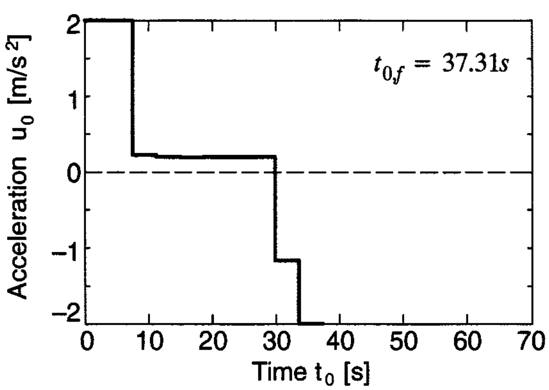

Figure 5. Car problem, optimal acceleration profile.

sense. Thus, the car problem clearly corresponds to the special bilevel optimization Problem SIOP6. The behavior of the car is described here using a nonlinear acceleration function and a friction term proportional to the square of the velocity. Mathematically, the resulting scenario-integrated dynamic optimization problem can then be stated as

$$\min_{a_0(t),\, t_{0,f}} \quad t_{0,f} \tag{23}$$

$$\begin{aligned}
\text{s.t.}\quad & \dot{v}_0(t_0) = \frac{4}{\pi}\arctan\big(a_0(t_0)\big) - k_f v_0^2(t_0), \quad v_0(t_{0,0}) = 0 \text{ m/s},\\
& \dot{d}_0(t_0) = v_0(t_0), \qquad d_0(t_{0,0}) = 0 \text{ m},\\
& v_0\big(t_{0,f}\big) = 0 \text{ m/s},\\
& d_0\big(t_{0,f}\big) = 300 \text{ m},\\
& v_0(t_0) \le 10 \text{ m/s},\\
& -2 \le a(t_0) \le 2,\\
& \forall t_0 \in \big[0, t_{0,f}\big],\\
& \dot{v}_1(t_1) = \frac{4}{\pi}\arctan(-0.2) - k_f v_1^2(t_1), \quad v_1(t_{0,1}^*) = v_0(t_{0,1}^*),\\
& \dot{d}_1(t_1) = v_1(t_1), \qquad d_1(t_{0,1}^*) = d_0(t_{0,1}^*),\\
& v_1\big(t_{1,f}\big) = 0 \text{ m/s},\\
& d_1(t_1) \le 350 \text{ m},\\
& \forall t_1 \in \big[t_{0,1}^*, t_{1,f}\big],\\
& \forall t_{0,1}^* \in \big[0, t_{0,f}\big].
\end{aligned}$$

In the sequel $k_f = 0.0025$ 1/m has been used for the reported computations. It has been assumed that the velocity and distance will not jump when the brakes fail such that mapping function $h_{0,1}$ reduces to continuity statements.

In a first step, the dynamic optimization problem for the car example is solved, without considering the possible brake failure. Therefore, only the upper set of constraints in Eq. 23 is considered. Dividing the time period into ten equally spaced intervals, the minimal time is calculated to be $t_{0,f} = 37.31$ s. The corresponding optimal acceleration profile is shown in Figure 5, and the trajectories of the velocity and the distance are depicted in Figure 6 (bold lines). In agreement with physical perception the car is accelerated as fast as possible until the speed limit is reached. Then the acceleration is reduced to a level that exactly equals the speed loss due to the friction term. This situation continues until the moment where the maximum brake force has to be applied in order to stop the car at 300 m with zero velocity. The intermediate values of the manipulated variables in the third and ninth intervals are only created by the discretization scheme, and vanish as the grid is refined or if the lengths of the discretization intervals are also optimized.

In order to analyze this result with respect to possible brake failure, dynamic simulations are now performed in a second step. Brake failures are assumed to occur only at the end of the discretization intervals. Starting at the instants $t_{0,1,k}^*$, the

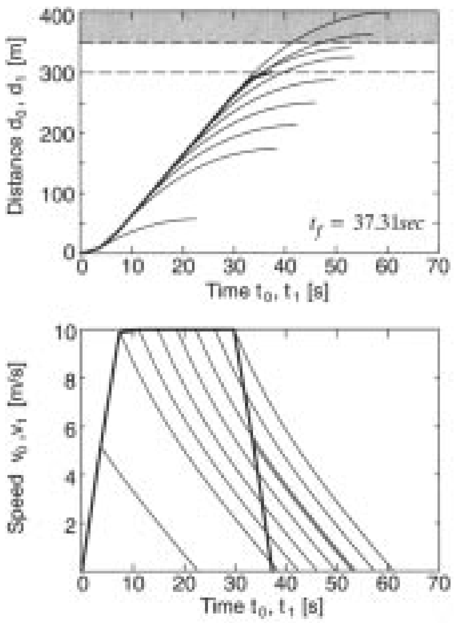

Figure 6. Car problem, covered distance (top) and speed (bottom).

Bold lines: nominal mode; thin lines: scenario mode.

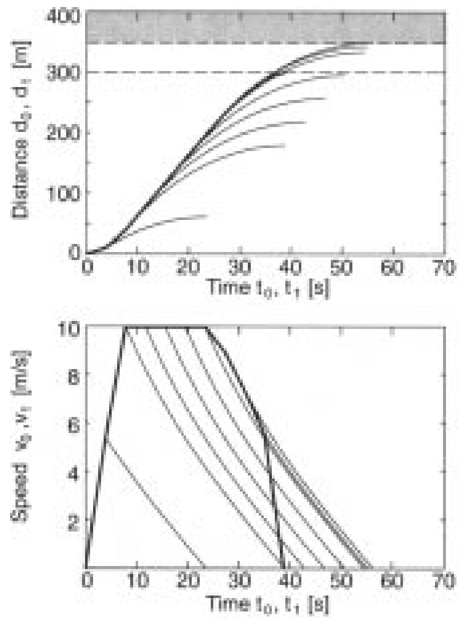

Figure 8. Car problem, covered distance (top) and speed (bottom) with distance constraint for the treated scenario.

Bold lines: nominal mode; thin lines: scenario mode.

scenario model is integrated until the car stops at $t_{1,f}$. The trajectories of the velocity and the distance resulting are also shown in Figure 6 (thin lines). Clearly, some of the trajectories in the upper part of the figure enter the shaded area, which indicates that the car will crash against the wall if the brakes fail during the time interval where these trajectories start.

This result is clearly unsatisfactory. Therefore, a scenario-integrated dynamic optimization problem 23 is now solved. The resulting optimal acceleration profile is shown in Figure 7. The corresponding trajectories of the covered distance and the velocity are depicted in Figure 8. Compared to Figure 5 the result has not changed qualitatively within the first 20 s. The car still reaches the speed limit as fast as possible and moves along this active constraint. But beginning at $t_0 \approx 23$ s, the speed is slowly reduced by taking into account the possible brake failure. The active constraint changes from the nominal speed limit to the distance of the scenario. This situation persists until the car stops at 300 m. The minimum time required to reach the desired endpoint has increased from $t_{0,f} = 37.31$ s to $t_{0,f} = 38.83$ s. However, the acceleration profile of Figure 7 is an inherently safe operational strategy and, being sure that the risk of injury due to brake failures is excluded, most car passengers would probably accept the slightly longer run time.

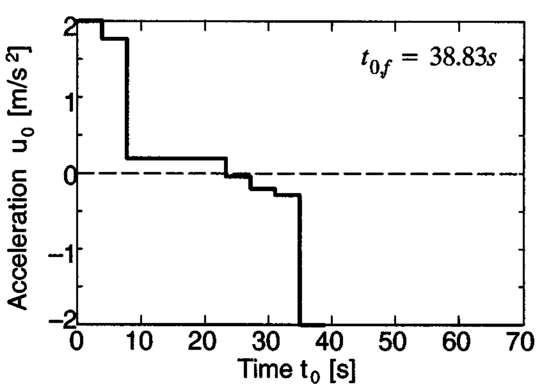

Figure 7. Car problem, optimal acceleration profile with distance constraint for the treated scenario.

Semibatch reactor

The second case study presented here corresponds to Example 3 discussed earlier. It deals with a semibatch reactor where the strongly exothermic consecutive reactions

$$A \rightarrow B \rightarrow C \tag{24}$$

take place. The reactor is shown in Figure 9. Initially, the vessel is supposed to be filled with a solvent. Then, component A is fed according to a specific recipe by adjusting the valve V. While the temperature should follow a desired profile, A reacts to B, which is partly consumed in order to form the undesirable component C. The reactor vessel is equipped with two heat-exchange systems, one acting through the reactor jacket (index j) and one using a coil inside the vessel (index c). Here the considered scenario is the possible failure of the jacket cooling system while the coil cooling system operates correctly. This still offers the possibility of driving the batch to an acceptable endpoint. However, the optimal operational profile for this scenario will probably differ from the optimal trajectories in the nominal mode.

Here, the model used for the semibatch reactor assumes that the system can be described by a single liquid phase and that the reaction kinetics are of first order. Neglecting changes in the concentrations due to the increasing volume of the reactor content, the following set of equations can be formatulated:

$$\dot{c}_a = \frac{F_a}{V_r} - k_{01} \exp\left(- \frac{E_1}{RT_r} \right) c_a, \tag{25}$$

$$\dot{c}_b = k_{01} \exp\left(- \frac{E_1}{RT_r} \right) c_a - k_{02} \exp\left(- \frac{E_2}{RT_r} \right) c_b, \tag{26}$$

$$\dot{c}_c = k_{02} \exp\left(- \frac{E_2}{RT_r} \right) c_b, \tag{27}$$

$$\dot{V}_r = \frac{F_a M_{Wa}}{\rho_r}, \tag{28}$$

$$\begin{aligned}(\rho_r c_{p_r}) \dot{T}_r = {} & \frac{F_a M_{Wa} c_{p_r}}{V_r} (T_f - T_r) \\ & - k_{01} \exp\left(- \frac{E_1}{RT_r} \right) c_a \Delta H_1 - k_{02} \exp\left(- \frac{E_2}{RT_r} \right) c_b \Delta H_2 \\ & + \alpha_{w,j} \frac{A_j}{V_{r,0}} (T_{w,j} - T_r) + \alpha_{w,c} \frac{A_c}{V_{r,0}} (T_{w,c} - T_r).\end{aligned} \tag{29}$$

The parameters are summarized in Table 1. These equations comprise component balances for the three species, a total mass balance, and an energy balance. In the latter, the temperatures inside the coil and the jacket are assumed to remain constant with varying flow through the cooling systems.

The objective of this study is to maximize the concentration of the desired product B at the endpoint of the batch by manipulating the quantities $F_a(t)$, $T_{w,j}(t)$, and $T_{w,c}(t)$. In the nominal mode the final time of the batch is fixed at $t_{0,f} = 6$ h. In addition, a single primary cooling system is assumed to provide the two heat exchangers with cooling medium such that the additional equation

$$T_{w,j,0} = T_{w,c,0} \tag{30}$$

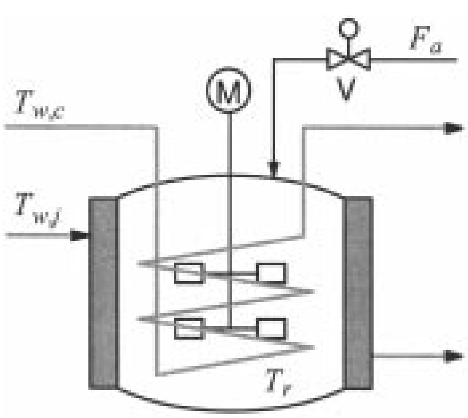

Figure 9. Treated semibatch reactor.

Table 1. Parameters for the Semibatch-Reactor Model

Parameter	Value	Parameter	Value
k_{01}	15.01 1/s	A_j	5.0 m^2
k_{02}	85.01 1/s	A_c	3.0 m^2
E_1	30,000.0 kJ/kmol	V_j	0.9 m^3
E_2	40,000.0 kJ/kmol	V_c	0.07 m^3
R	8.314 kJ/kmol/K	$V_{r,0}$	1.0 m^3
M_{W_a}	50.0 kg/kmol	ρ_w	700.0 kg/m^3
ρ_r	1,000.0 kg/m^3	c_{p_w}	3.1 kJ/kg/K
c_{p_r}	3.9 kJ/kg/K	$c_a(t_{0,0})$	0.0 kmol/m^3
T_f	300.0 K	$c_b(t_{0,0})$	0.0 kmol/m^3
ΔH_1	$-40{,}000.0$ kJ/kmol	$c_c(t_{0,0})$	0.0 kmol/m^3
ΔH_2	$-50{,}000.0$ kJ/kmol	$T_r(t_{0,0})$	300.0 K
$\alpha_{w,j}$	0.8 kJ/s/m^2/K	$V_r(t_{0,0})$	1.0 m^3
$\alpha_{w,c}$	0.7 kJ/s/m^2/K		

is stated, reducing the number of operational degrees of freedom in the nominal mode to two. The endpoint constraints in this mode comprise a fixed amount of added feed and an upper limit on the educt concentration c_a. Furthermore, the temperature must be limited for the case of a total cooling system failure during the batch. In principle, this situation could be considered as an additional scenario. However, no operational degree of freedom would be available in that case, and the problem would then resemble the car problem treated in the previous subsection. In addition, the scenario ''total loss of cooling capacity'' can be incorporated more simply by applying the concept of the adiabatic end temperature (Abel et al., 1999; Stoessel, 1995; Ubrich et al., 1999). For the system composed of the reactor and the two heat exchangers, this expression can be calculated from a stationary energy balance, yielding

$$T_{ad} = T_r + \frac{V_r[(-\Delta H_1 - \Delta H_2) c_a + (-\Delta H_2) c_b]}{\rho_r c_{p_r} V_r + \rho_w c_{p_w} (V_j + V_c)}. \tag{31}$$

The process model for the nominal mode comprises Eqs. 25 to 31. It contains $n_0 = 5$ differential variables, $m_0 = 2$ algebraic variables, and $p_0 = 2$ operational degrees of freedom.

If the jacket cooling system fails, Eq. 30 no longer holds. It must then be replaced by an energy balance for the reactor jacket:

$$(\rho_w c_{p_w} V_j) \dot{T}_{w,j} = \alpha_{w,js} A_j \frac{V_r}{V_{r,0}} (T_{w,j} - T_r). \tag{32}$$

The heat exchange between the jacket wall and the contents of the reactor will now be considerably smaller than in the nominal mode, due to the missing flow of cooling medium through the jacket. This is modeled by choosing a reduced value for the heat transfer coefficient $\alpha_{w,js} = 0.3$ kJ/s/m^2/K. These changes lead to $n_1 = 6$ differential variables and $m_1 = 1$ algebraic variables, such that the process models for the nominal and the scenario modes are parametrically and structurally different. The mapping $h_{0,1}$ between the state variables of these models at switching times $t^*_{0,1}$ reduces to continuity equations for the five differential variables of the nominal mode. The additional differential variable in the scenario mode, $T_{w,j,1}$, is initialized with the value of the same variable in the nominal mode, which is here one of the algebraic variables. Thus, $h_{0,1}$ can be stated as

$$[c_{a,1}, c_{b,1}, c_{c,1}, V_{r,1}, T_{r,1}]^T_{t^*_{0,1}} = [c_{a,0}, c_{b,0}, c_{c,0}, V_{r,0}, T_{r,0}]^T_{t^*_{0,1}}, \tag{33}$$

$$T_{w,j,1}(t^*_{0,1}) = T_{w,j,0}(t^*_{0,1}). \tag{34}$$

Although one of the cooling systems has failed in the scenario mode, it will be assumed in the sequel that the main operational goal during this process phase is still the maximization of the product concentration c_b, which can be achieved by manipulating the feed flow rate and the temperature of the coil cooling system. As long as it can be ensured that the total loss of cooling energy does not cause any severe problem, this situation may be realistic, in particular for high-value products where the loss of a batch must be avoided. Consequently, the objective function and the constraints of the scenario mode are identical to those in the nominal mode. The final time in the scenario will, however, not be fixed. It is instead regarded as an operational degree of freedom to be determined as solution of the scenario-integrated dynamic optimization problem with an upper limit of $t_{1,f} \le t^*_{0,1} + 6h$.

In this configuration, the optimization problem for the semibatch reactor must be classified as a single-level optimization problem of the type shown in Problem SIOP2. Summarizing the details, and providing the problem-specific data, it can be mathematically formulated as

$$\min_{\substack{F_{a,0}(t_0),\, T_{w,c,0}(t_0),\\ F_{a,1}(t_1),\, T_{w,c,1}(t_1),\, t_{1,f}}} \quad -0.9 c_{b,0}(t_{0,f}) - 0.1 \int_0^{6h} c_{b,1}(t_{1,f})\, dt^*_{0,1} \tag{35}$$

s.t. f_0: Eqs. 25 to 31 in t_0 and with variable index 0,

$$g_0: \int_0^{6h} F_{a,0}\, dt_0 = 20 \text{ kmol},$$

$$c_{a,0}(t_{0,f}) \le 0.5 \text{ kmol},$$

$$T_{ad,0}(t_0) \le 453 \text{ K},$$

$$0 \le F_{a,0}(t_0) \le 180.0 \text{ kmol/h},$$

$$288 \text{ K} \le T_{w,c,0}(t_0) \le 432 \text{ K},$$

$$\forall t_0 \in [0, 6h],$$

f_1: Eqs. 25 to 29 and Eq. 31 in t_1 and with variable index 1,

$h_{0,1}$: Eqs. 33 and 34,

$$g_1: \int_0^{t^*_{0,1}} F_{a,0}\, dt_0 + \int_{t^*_{0,1}}^{t_{1,f}} F_{a,1}\, dt_1 = 20 \text{ kmol},$$

$$c_{a,1}(t_{1,f}) \le 0.5 \text{ kmol},$$

$$T_{ad,1}(t_1) \le 453 \text{ K},$$

$$0 \le F_{a,1}(t_1) \le 180.0 \text{ kmol/h},$$

$$288 \text{ K} \le T_{w,c,1}(t_1) \le 432 \text{ K},$$

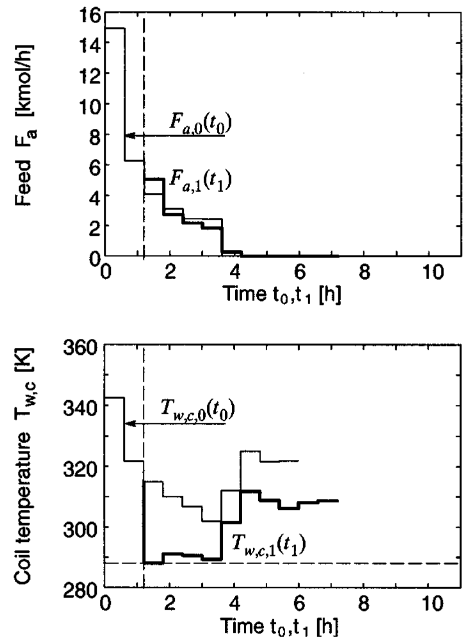

Figure 10. Free operational variables of the semibatch reactor for a failure of the jacket cooling system at $t^*_{0,1} = 1.2$ h.

Bold lines: scenario mode; thin lines: nominal mode.

$$0 \text{ h} \le t_{1,f} - t^*_{0,1} \le 6 \text{ h},$$

$$\forall t_1 \in [t^*_{0,1}, t_{1,f}],$$

$$\forall t^*_{0,1} \in [0, 6h].$$

Problem 35 is solved with the time period for the nominal mode divided into 10 intervals. Scenarios are again assumed to start only at the resulting discretization points and their time horizons are also divided into 10 elements. For reasons of brevity, results are given here only for scenarios starting at $t^*_{0,1} = 1.2$ h, $t^*_{0,1} = 3.0$ h, and $t^*_{0,1} = 4.8$ h. They show all the interesting features without occupying too much space.

The free operational variables, comprising the feed flow rates $F_{a,0}(t_0)$ and $F_{a,1}(t_1)$, as well as the cooling temperatures $T_{w,c,0}(t_0)$ and $T_{w,c,1}(t_1)$, for the case where the jacket cooling system fails at $t^*_{0,1} = 1.2$ h are depicted in Figure 10. The optimal trajectories for the nominal mode are drawn in thin lines and the results for the scenario mode are presented in bold lines. As can be seen in the upper part of the figure, the feeding profiles for component A in the nominal and the scenario modes differ only slightly. On the other hand, the necessary coil temperature in the lower part of Figure 10 decreases considerably in the scenario mode compared to the temperature chosen for both systems in the nominal mode. It nearly reaches the lower limit of $T_{w,c,\min} = 288$ K, drawn in a dashed line in the figure.

Figure 11 shows the trajectories of the state variables of interest that correspond to the optimal operational profile of Figure 10. The upper part of Figure 11 shows the reactor temperature and the adiabatic end temperature defined by Eq. 31. Whereas the temperature for the scenario is chosen

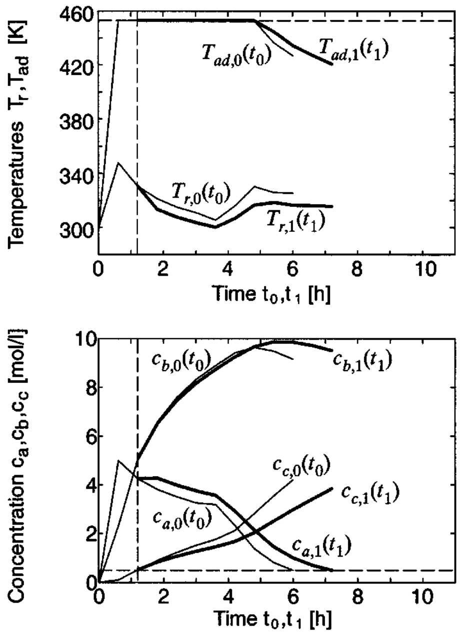

Figure 11. Constrained variables of the semibatch reactor for a failure of the jacket cooling system at $t^*_{0,1} = 1.2$ h.

Bold lines: scenario mode; thin lines: nominal mode.

to be lower than for the nominal mode, the adiabatic end temperature is the active constraint of the process in both discrete modes. This result does not surprise, since such a safety constraint was already earlier found to be the limiting factor for the optimization of exothermic semibatch reactors (Abel et al., 1999; Ubrich et al., 1999).

The concentration profiles of the three components appear in the lower part of Figure 11. Qualitatively, the result for the nominal and the scenario modes are similar. Initially, the amount of A in the reactor rises and the conversion to B immediately starts, followed by the consecutive reaction to C with a delay of about 0.5 h. After the first discretization interval, the educt concentration continuously decreases until the desired endpoint value of $c_{a,0}(t_{0,f}) = c_{a,1}(t_{1,f}) = 0.5$ mol/L is reached. The amount of product B rises during most of the batch, although a decrease at the end has to be tolerated in order to fulfill the endpoint constraint for c_a. It is interesting to note that the final product concentration at the end of the scenario mode, $c_{b,1}(t_{1,f}) = 9.51$ mol/L, is higher than that at the end of the nominal mode, $c_{b,0}(t_{0,f}) = 9.15$ mol/L. This is due to the fact that the optimal duration of the scenario mode was found to be a maximum of 6 h. The complete scenario batch time is therefore equal to 7.2 h, which is longer than the nominal batch time used here. If an optimization problem is solved only for the nominal batch with a fixed final time of $t_f = 7.2$ h divided into 11 elements, an optimal value of $c_b(t_f) = 9.51$ mol/L is also found (results not shown here).

The trajectories for a failure of the jacket cooling system at time $t^*_{0,1} = 3.0$ h are shown in the Figures 12 and 13. The feed flow rate of the first time interval after the scenario has started is now exactly the same as in the nominal mode. The average temperature level for the remaining coil cooling system has decreased further in the scenario mode compared to Figure 10. The adiabatic end temperature is still the active constraint of the optimal profile of both modes. The duration

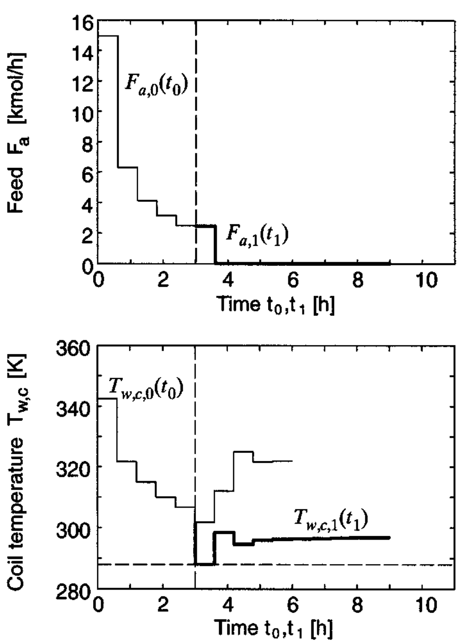

Figure 12. Free operational variables of the semibatch reactor for a failure of the jacket cooling system at $t^*_{0,1} = 3.0$ h.

Bold lines: scenario mode; thin lines: nominal mode.

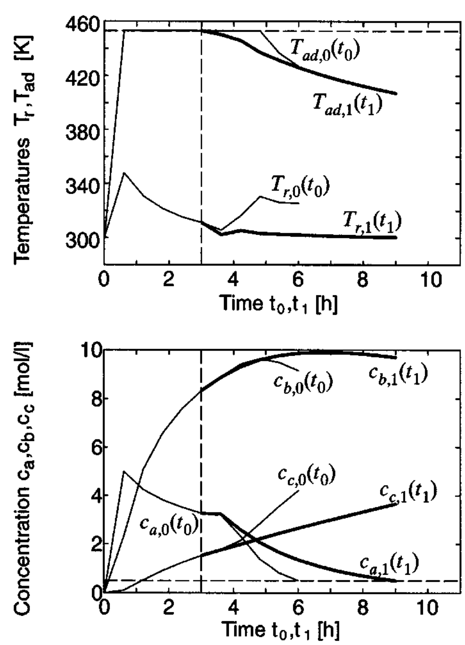

Figure 13. Constrained variables of the semibatch reactor for a failure of the jacket cooling system at $t^*_{0,1} = 3.0$ h.

Bold lines: scenario mode; thin lines: nominal mode.

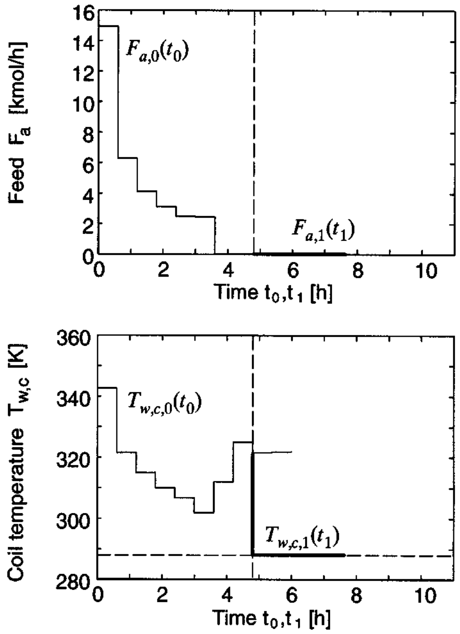

Figure 14. Free operational variables of the semibatch reactor for a failure of the jacket cooling system at $t^*_{0,1} = 4.8$ h.

Bold lines: scenario mode; thin lines: nominal mode.

of the scenario is again chosen to be 6 h, such that in this case, the total batch duration is 9 h. The final product concentration in the scenario even reaches a value of $c_{b,1}(t_{1,f}) = 9.70$ mol/L.

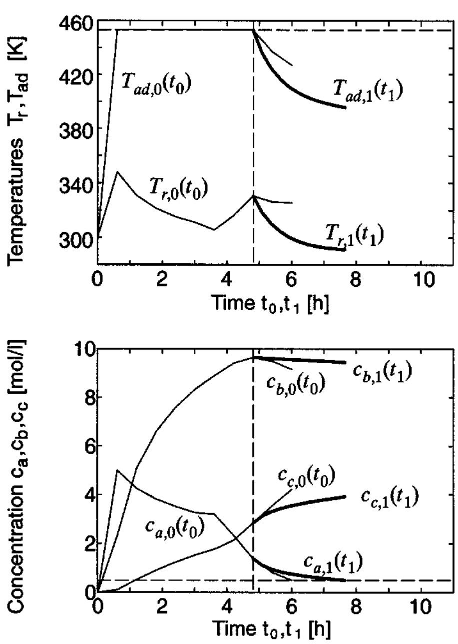

Figure 15. Constrained variables of the semibatch reactor for a failure of the jacket cooling system at $t^*_{0,1} = 4.8$ h.

Bold lines: scenario mode; thin lines: nominal mode.

Table 2. Duration and Final Product Concentration of the Scenarios in Problem 35

$t^*_{0,1}$	$t_{1,f} - t^*_{0,1}$	$c_{b,1}(t_{1,f})$
0.6 h	6.00 h	9.37 mol/L
1.2 h	6.00 h	9.51 mol/L
1.8 h	6.00 h	9.61 mol/L
2.4 h	6.00 h	9.66 mol/L
3.0 h	6.00 h	9.70 mol/L
3.6 h	6.00 h	9.76 mol/L
4.2 h	5.93 h	9.78 mol/L
4.8 h	2.85 h	9.44 mol/L
5.4 h	1.05 h	9.25 mol/L
6.0 h	0.02 h	9.15 mol/L

The last instant for a failure of the jacket cooling system to be discussed here is $t^*_{0,1} = 4.8$ h, and the results obtained for this case are shown in Figures 14 and 15. At $t_0 = 4.8$ h, component A has already been completely added to the reactor such that this scenario corresponds to a pure batch process. The optimal operation of these processes can be derived analytically or geometrically for a number of possible kinetic schemes (Rippin, 1983). For the case treated here—a consecutive reaction with the activation energies related according to $E_{A\rightarrow B} < E_{B\rightarrow C}$—a decreasing temperature profile is recommended. This is exactly what has been determined through the solution of Problem 35 for the scenario starting at $t^*_{0,1} = 4.8$ h. Here, the duration of the scenario was calculated to be 2.85 h, which is significantly shorter than the maximum value. The final value of the product concentration reaches $c_{b,1}(t_{1,f}) = 9.44$ mol/L, which is lower than in the scenario starting at $t^*_{0,1} = 3.0$ h. This can be explained easily by the fact that all the feed already has been added here such that the possibilities of increasing the product concentration further are restricted.

In order to present at least the most interesting process variables for all the scenarios treated, the duration $t_{1,f} - t^*_{0,1}$ and the final product concentration $c_{b,1}(t_{1,f})$ of the different scenarios in Problem 35 are summarized in Table 2. Clearly, the batch time is chosen to be as long as possible for the scenarios starting at points where a significant amount of feed is still to be added. For later failures of the jacket cooling system this time period is continually reduced until zero is nearly reached for the last considered scenario. (Since the final time is treated as additional parameter of the optimization problem, all differential equations are multiplied by this variable. For numerical reasons the lower limit on the final time must therefore always remain nonzero. Here, a bound of $t_{1,f,\min} = 0.02$ h has been used.) This would indeed be expected, since the endpoint is already optimal for all the constraints being fulfilled, and a longer batch time would only lead to increased production of the unwanted product C.

Conclusions

In this article scenario-integrated modeling and optimization of dynamic systems have been introduced. This new class of problems allows the study of chemical processes during transient phases, including their behavior after the occurrence of certain scenarios. The formulated models are of a hybrid (discrete-continuous) nature and possess a special structure where the transitions between the nominal mode and the scenario modes are only monodirectional. Since the time instant of an event is assumed to be unknown, any instant on the time horizon of the nominal mode must be treated as a possible switching time, resulting in the simultaneous analysis of the system along multiple time axes.

Two major problem classes have been discussed for the scenario-integrated optimization of dynamic systems. One aims predominantly at minimizing a chosen objective function in all the existing discrete modes of the system. This problem can be interpreted as an extension of stochastic optimal control problems. In contrast to the latter class, which determines a single operational strategy that is robust against all existing uncertainties, the solution of scenario-integrated optimization problems comprise different profiles of the controlvariables for the various switching times. Furthermore, scenario-specific models and constraints are possible. The second problem formulation assumes that a qualitative difference exists between the objective in the nominal operation and those in the scenario modes. This assumption results in a dynamic bilevel optimization problem where the optimization problems for the scenario modes restrict the problem in the nominal mode.

The derived problem formulations are very complex. Nearly all related areas ranging from hybrid systems over stochastic programming to embedded optimal control problems, the theoretical analysis and the development of numerical solution techniques are subjects of current research. Therefore, solution techniques could only be developed for restricted subclasses of the formulated problems. These cases comprise single-level optimization problems with only one layer of scenario modes and bilevel optimization problems without operational degrees of freedom in the scenarios. In the approach presented, an approximate solution of these problems is achieved by replacing the infinite number of possible switching times to the scenario modes by a finite number of examined transitions. These transitions have to be placed sufficiently close in the nominal time period to limit constraint violations for switching times not explicitly treated to an acceptable extent. The resulting technique has been applied to two examples that deal with the integration of safety into transient process design.

The results obtained in this article motivate a number of future research activities. Above all, these activities include the theoretical analysis of the derived scenario-integrated optimization problems. In particular, problems with multiple subsequent transitions over a number of discrete modes must be investigated. The numerical solution techniques have to be improved for all scenario-integrated dynamic optimization problems. Here, the possibilities for the single-level problems include the application of advanced integral sampling techniques. Both problem classes may profit from the exploitation of the problem structure, for example, within a parallel computing environment. The resulting reductions in computational times may then allow the real-time solution of scenario-integrated optimization problems, an area that has had little attention so far (Abel and Marquardt, 1998). The developed theory may finally be applied to a broader range of problems in order to provide solutions for the optimal operation of chemical processes under a wide variety of existing uncertainties.

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