PARAMETER ESTIMATION OF AN INDUSTRIAL EVAPORATOR WITH HYBRID DYNAMICS BY A SMOOTHING APPROACH

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Keywords: Parameter estimation, Dynamic optimization, Hybrid systems, Smoothing method.

Abstract: Evaporation systems are essential in process industries. Due to phase transitions and changes of operating modes these systems has to be classified as hybrid systems and the simulation and optimization based on detailed models is often a challenging if not an intractable task. In this study we apply a smoothing approach in order to modify the hybrid model such that the discrete transitions are integrated into a system of differential algebraic equations leading to exclusively smooth trajectories. The simulation results of the smooth model are compared to those of the original hybrid model. With a view to parameter estimation the sensitivity with respect to the smoothing parameter as well as the parameters to be estimated are calculated. The parameter estimation is carried out for the smooth model and the dependence of the optimization results on the smoothing parameter is investigated.

1 INTRODUCTION

Nowadays, simulation and optimization based on physical models are indispensable tools to improve design and operation of complex industrial systems. Optimization problems occur for many tasks such as parameter estimation, data validation, safety verification and model predictive control. The objective of the respective optimization is subject to the dynamic model equations of the process under consideration and possibly to additional equality and inequality constraints resulting, e.g., from safety demands. State-of-the-art methods allow for successfully solving optimization problems which include only continuous system models expressed as a set of differential algebraic equations (DAE). However, in many fields, e. g., chemical processes, power plants, oil refineries, continuous and discrete state dynamics are coupled strongly. Such systems with mixed continuous and discrete dynamics are called hybrid systems. The discrete dynamics result from instantaneous autonomous or controlled (externally triggered) transitions from one operating regime to another. Between these transition points, the state variables of the system evolve continuously according to the DAE of the respective operation mode. Due to the mixed discrete-continuous dynamics, the trajectories of the state variables are in general non-smooth or even discontinuous, which may impede the optimization of such systems. Several approaches, e.g., mixed-integer programming, heuristic methods, relaxation and penalization strategies have been proposed to tackle this problem. Since relaxation strategies are most promising with regard to the computation time, they will be studied in this paper. Up to now mostly relatively small systems have been studied using relaxation methods. In this study, a large-scale industrial evaporator with switching behavior is formulated as a hybrid model and as a relaxed continuous model, respectively. Both models are simulated and the parameter sensitivities are calculated over the whole time horizon. For the smooth model, results of the parameter estimation and the dependence of the solution on the reformulation parameter are shown.

The paper is organized as follows. The challenges and solution approaches for simulation and optimization of hybrid dynamic systems are discussed in Section 2. Section 3 presents the evaporator model in its hybrid and relaxed form. In Section 4, the simulation results of the relaxed (and consequently smooth continuous) model are compared with those of the original hybrid model. Section 5 applies our smoothing

Mynttinen I., Runge E. and Li P..
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DOI: 10.5220/0003575500310036
In *Proceedings of 1st International Conference on Simulation and Modeling Methodologies, Technologies and Applications* (SIMULTECH-2011), pages 31-36
ISBN: 978-989-8425-78-2

method to two fundamental tasks of process engineering, namely parameter estimation and the calculation of sensitivities. Section 6 summarizes the results and concludes the paper.

2 OPTIMIZATION OF HYBRID SYSTEMS

Mathematically, discrete transitions in hybrid systems are often formulated in terms of complementarity conditions. In actual numerical simulation, discrete transitions are almost always handled through embedded logical statements. At the zero-crossing points of some switching function, the initial conditions are updated and the appropriate set of equations is solved restarting at this point in time (Barton and Lee, 2002). Systems with so-called Filippov solutions that remain for a while at the zero-crossing require additional analysis. Since they do not pose a particular problem for our approach, we will not discuss them further here. A profound analysis and numerical simulation results of hybrid systems can be found in (Mehrmann and Wunderlich, 2009; Goebel et al., 2009). For optimization tasks, the hybrid simulation can be embedded into a heuristic search algorithm. For instance, particle swarm optimization has been applied by (Pappala and Erlich, 2008) to the unit commitment problem. These methods suffer from high computational cost when many function evaluations are needed (i.e. in a high dimensional search space). Alternatively one can consider the problem as a constrained optimization problem subject to the dynamic model equations. This leads to a dynamic nonlinear program (NLP). In the so-called direct method, the DAE system is discretized resulting in a large-scale NLP with equality (and possibly inequality) constraints, which can be solved by means of a NLP solver with a gradient-based search. However this NLP-based optimization of hybrid systems is an extremely challenging task due to the non-smoothness of the objective function or constraints which result from instantaneous mode transitions. As a consequence, NLP regularity cannot be presumed and NLP solvers may fail. Essentially three different approaches can be used to overcome this difficulty. Mixed-integer methods have been applied successfully to optimal control problems by (Sonntag et al., 2006) and (Barton et al., 2006), where a graph search algorithm explores the state space of the discrete variables. An embedded NLP is used to find the local optima in the continuous state space. The complexity study in (Till et al., 2004) indicates that for systems with many decision variables solving the problem becomes computationally expensive. The second approach applied, e.g., by (Prada et al., 2007) and (Voelker et al., 2007) comprises sequential optimization methods. Here, the optimization layer exclusively contains continuous variables. The hybrid system is put into the simulation layer and solved by any simulator which is capable to treat discontinuities. Again, the necessity of many simulation runs increases the computational cost. Reformulation strategies, which represent the third class of methods, introduce additional variables and parameters to remove the non-smoothness related to the complementarity conditions from the problem while retaining the desired features. Reformulation strategies have been studied by (Baumrucker et al., 2008; Sager, 2009; Ralph and Wright, 2004). Most reformulation strategies fall into one of the following two classes: (i) Relaxation methods transform the complementarities into a set of relaxed equality or inequality constraints, e.g., by the smoothing discussed in this contribution. A sequence of relaxed problems is solved in order to approach the solution of the original problem. (ii) Penalization methods introduce a penalization term into the objective function which measures the violation of the complementarity condition.

3 MODEL OF THE EVAPORATOR

The evaporation of volatile components to concentrate non-volatile components within a mixture is a common technology in process engineering. Usually multi-stage systems built up from several identical single evaporators are used. Such a single evaporator model is considered in this paper following (Sonntag et al., 2006). The system consists of an evaporation

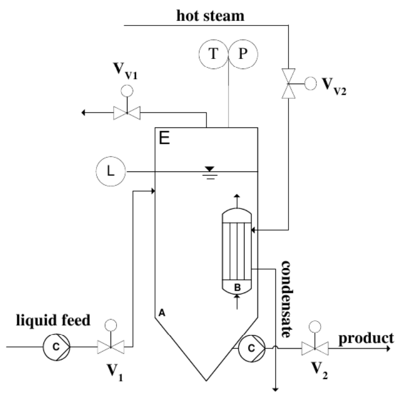


Figure 1: Evaporator model (Sonntag et al., 2006).

tank and a heat exchanger (see Figure 1). The tank is fed through the valve V_1 with a mixture of three liquid components A, B, C with mass fractions w_A, w_B, w_C, where A is a hydrocarbon of high molar mass and thus has a very low vapor pressure (implemented as $P_A^0 = 0$ in the model) compared to water (B) and ethanol (C). Inside the tank, the volatile components are evaporated. Hence the mass fraction of the non-volatile component A in the liquid is increased. This product will be drained from the tank through the valve V_2 when the desired concentration of A is reached. The vapor which consists of B and C with the mass fractions ξ_B, ξ_C determined by the phase equilibrium escapes from the tank through the valve V_{v1}. In order to heat the tank, hot vapor is supplied to the heat exchanger, where the vapor condensates and leaves the heat exchanger as a liquid.

Depending on the pressure inside the evaporator and the temperature difference between the heat exchanger and the tank, $M = 4$ operating modes can be distinguished: If the temperature of the heat exchanger is higher than that of the tank, the heat exchanger operates in the mode 'heating' (H), otherwise 'non-heating' (NH). Inside the tank, the transition from the mode 'non-evaporating' (NE) to the mode 'evaporating' (E) occurs as soon as the pressure reaches a certain threshold. Hence, during operation the system may visit the four operating modes: NE/NH ($m = 1$), NE/H ($m = 2$), E/H ($m = 3$) and E/NH ($m = 4$). Thus, the evaporator model possesses the typical features of a hybrid system with autonomous mode transitions.

3.1 The Hybrid Evaporator Model

The hybrid model of the evaporator consists of four sets of DAE $f^{(m)}(\dot{x}, x, p) = 0$, $m = 1, \ldots, M$ which can be found in (Sonntag and Stursberg, 2005). The tank and the heat exchanger change their operation mode when the respective state-dependent switching function $\psi^{(1)}(p) = p - p_c$, $p_c = 0.4\,\text{bar}$ or $\psi^{(2)}(T) = T - T_{heatex}$ crosses 0. T and p denote the temperature and the pressure in the tank. As a consequence of this zero-crossing, the dynamics change and the state variables immediately before the switch x^- have to be mapped onto the state variables immediately after the switch x^+ using the so-called transition functions $x^+ = \mathcal{T}(x^-)$. For instance, for the vapor mass fraction ξ_B the transition function from the non-evaporating modes ($m = 1, 2$) to the evaporating modes ($m = 3, 4$) reads

$$\xi_B^+ = \xi_B^- + \frac{w_B P_B^0(T)}{w_A P_A^0(T) + w_B P_B^0(T) + w_C P_C^0(T)} \qquad (1)$$

with the temperature $T^+ = T^- = T$ and the liquid mass fractions $w^+ = w^- = w$.

3.2 A Smooth Evaporator Model

State trajectories are in general non-smooth or even discontinuous at the transition points. If such a model is included into an optimization problem, these points are severe obstacles for gradient-based optimization algorithms. In order to make the optimization of hybrid systems accessible to NLP solvers, the complementarity condition of the original problem is relaxed, i.e., the strict complementarity conditions are fulfilled only approximately. In our smoothing approach, we replace the if-else-statement by the smoothing function

$$\varphi(x) = \left(1 + \exp\left[-\frac{\psi(x)}{\tau}\right]\right)^{-1} \qquad (2)$$

with the small smoothing parameter τ. The model equations are combined in one single set of equations according to

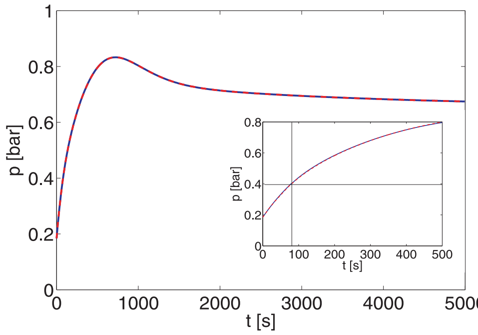
$$\begin{aligned} f(\dot{x}, x, p) = {} & \varphi(x)\, f^{(1)}(\dot{x}, x, p) \\ & + (1 - \varphi(x))\, f^{(2)}(\dot{x}, x, p). \end{aligned} \qquad (3)$$

This reproduces the switching behavior of the hybrid model in the limit $\tau \to 0$.

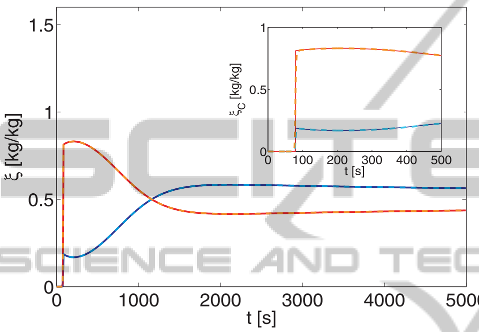
4 SIMULATION RESULTS

Figure 2 shows that the trajectories of the smooth model with smoothing parameter $\tau = 0.002\,\text{bar}$ and of the original hybrid model deviate only marginally from each other. When the pressure meets the transition condition $p = p_c$ (see inset of Figure 2(a)) the evaporator switches from the non-evaporating mode to the evaporating mode. As a consequence, the mass fractions of the volatile components B and C jump according to Eq. 1 from 0 in the non-evaporating mode (no vapor is present) to the finite values given by the phase equilibrium (see Figure 2(b)) and vapor starts to escape from the tank (Figure 2(c)). The evaporation of the volatile components B and C leads to a decrease of their mass fractions w_B, w_C in the liquid. The decrease of w_C (ethanol) is more pronounced due to the higher vapor pressure and thus the higher outflow of C. Consequently, the vapor mass fractions cross each other near $t = 1150\,\text{s}$ (Figure 2(b)). Since the pressure in the evaporator and also the vapor outflow (Figure 2(a) and 2(c)) depend on the (temperature-dependent) vapor pressure and the mass fractions of all liquid components, both first increase due to the increasing temperature and later decrease due to the reduced mass fractions w_B, w_C in the liquid.

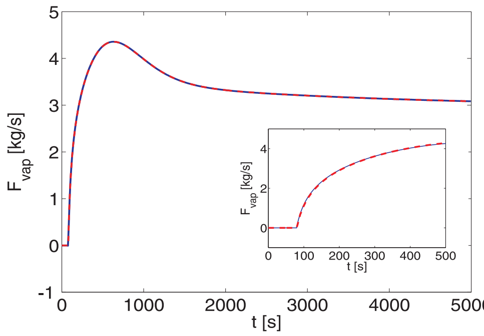
Figure 3 demonstrates that the smooth model approximates the hybrid model the better the smaller



(a) Pressure inside the evaporator for the hybrid model (blue) and the smooth model (red).



(b) Mass fractions of the volatile components B (hybrid model: dark blue, smooth model: light blue) and C (hybrid model: red, smooth model: orange) in the vapor.



(c) Vapor flow from the evaporator for the hybrid model (blue) and the smooth model (red).

Figure 2: Simulation results of the hybrid and the smooth model.

the smoothing parameter τ is chosen: The slope of the state trajectory ξ_C increases and the transition region narrows. In the transition region, the dynamics is given by the linear combination (Eq. 3) of both operation modes involved. It is important to note that the trajectories of the hybrid model and the smooth approximation are nearly identical outside the transition region. Obviously, the smoothing only extends the transition time but does not drive the system to a different region of the state space. From this result we conclude that the smoothing approach is well suited

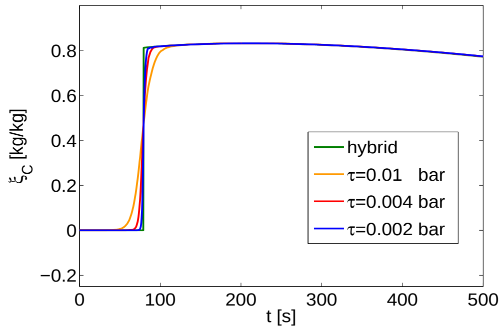


Figure 3: Mass fraction ξ_C from simulations with several values of the smoothing parameter.

for the evaporator model.

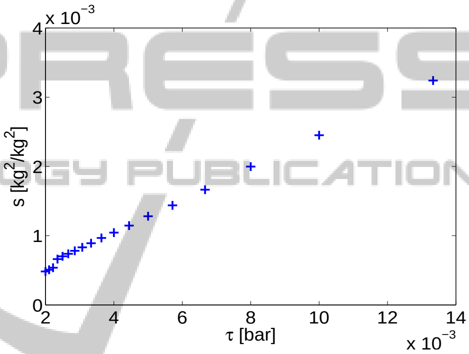


Figure 4: Deviation of the smooth model from the hybrid model as a function of the smoothing parameter.

For a more quantitative analysis of the convergence of the solutions of the relaxed model to that of the original model, we consider in Figure 4 the average squared deviation

$$s = \frac{1}{N}\sum_{i=1}^{N}\left[\xi_C^{(hybrid)}(t_i) - \xi_C^{(smooth)}(t_i)\right]^2 \qquad (4)$$

between the vapor mass fractions ξ_C calculated with the hybrid and the smooth model. The average squared deviation is found to follow approximately $s \propto \tau$ and is dominated by the finite width of the transition region.

5 PARAMETER ESTIMATION AND SENSITIVITY ANALYSIS

A fundamental task frequently occurring in process engineering is parameter estimation. Parameter estimation in general aims at extracting the best guesses of the parameters determining the dynamics of the system under consideration based on a series of measurements $x_{ij}^{(m)}$ of several state variables x_i, $i = 1,\dots,M$ at different points in time t_j, $j = 1,\dots,N$. It is useful to combine the parameter estimation of a hybrid system with the sensitivity analysis for at least two reasons: First, the sensitivities of the measured state variables with respect to the parameters to be estimated allow to evaluate the applicability of certain data in a parameter estimation problem. Second, the sensitivity with respect to the smoothing parameter is needed to predict the suitability of the smooth model for parameter estimation. The sensitivity of the state variable ξ_C with respect to the smoothing parameter (Figure 5) quantifies the observation already stated qualitatively in Section 4 that the influence of the smoothing is restricted to the transition region, i.e., $\frac{d\xi}{d\tau} \approx 0$ outside. The shape of $\frac{d\xi_C}{d\tau}$ is easily understood in view of the trajectory shown in Figure 3. As τ increases, i.e., $\Delta\tau = \tau_2 - \tau_1 > 0$, the curve $\xi_C(\tau_2)$ lies above that of $\xi_C(\tau_1)$ as long as $p < p_c$ and thus $\Delta\xi_C = \xi_C(\tau_2) - \xi_C(\tau_1)$ is negative, whereas it is positive when $p > p_c$. In Figure 5, the sensitivity is calculated at the rather large parameter value $\tau = 0.01\,$bar. A smaller τ yields narrower regions with $\frac{d\xi}{d\tau} \neq 0$ (not shown).

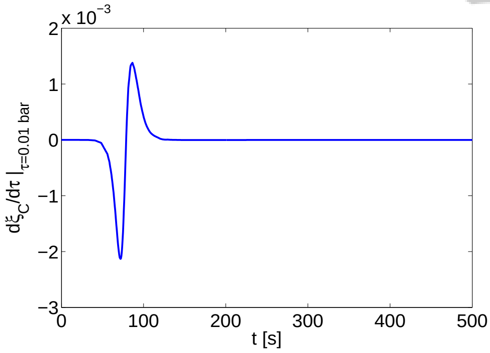
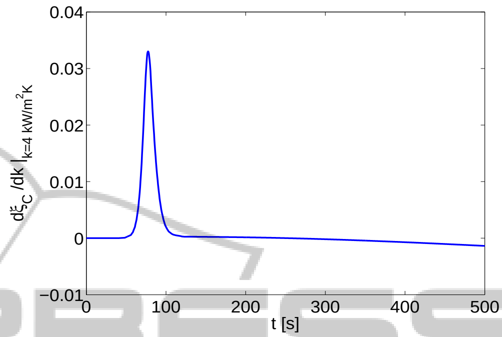
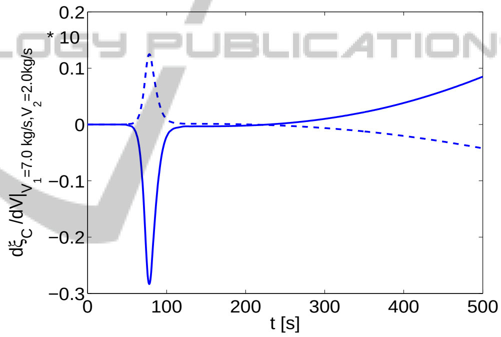


Figure 5: Sensitivity with respect to the smoothing parameter.

Below, we will estimate the coefficient k of the heat transfer from the heat exchanger to the tank, the valve throughputs of the liquid inflow (V_1) and the liquid outflow (V_2) based on measurements of the ethanol vapor mass fraction ξ_C. This choice of the measured variable is due to the fact that ξ_C is one of the quantities with the most significant hybrid behavior, which shows up as a jump at the mode transition (Figure 2(b)). As can be seen in Figure 6, the corresponding sensitivities are relatively large around the mode transition. The most dominant influence of the heat transfer and the liquid in- and outflow, i.e., the mass of liquid to be heated is indirect via the transition time NE $\rightarrow$ E. An increase of the heat transfer coefficient or a decrease of the liquid inflow shifts the curve $\xi_C(t)$ to the left, i.e., accelerates the process. Hence the respective sensitivities are positive and negative in the first time period and change sign when $\xi_C(t)$ exceeds its maximum. Based on Figure 6, one can expect to find the correct parameter values by means of parameter estimation, if ξ_C data are available around the transitions or in the late time period.



(a) Sensitivity with respect to the heat transfer coefficient.



(b) Sensitivity with respect to the valve throughputs (liquid inlet: solid, liquid outlet: dashed).

Figure 6: Sensitivities of the mass fraction of component C.

The 'measurement data' for our parameter estimation have been generated by simulation of the hybrid system with added Gaussian distributed measurement error ($\sigma = 0.04\,kg/kg$). We use a series of 51 equidistant data points within the time horizon $t \in [0, 500]\,$s. As usual, the parameter estimation problem is formulated as least-square optimization. Figure 7 shows the simulation results of the hybrid model and the optimization result for a particular realization of 'measurement data'. The corresponding optimal parameter values ($k^{(opt)} = 4.070\,kW/m^2K$, $V_1^{(opt)} = 6.968\,kg/s$ and $V_2^{(opt)} = 1.950\,kg/s$) agree very well with the values used for the data generation ($k^{(opt)} = 4.0\,kW/m^2K$, $V_1^{(opt)} = 7.0\,kg/s$ and $V_2^{(opt)} = 2.0\,kg/s$). The optimal parameters are quite robust regarding the smoothing parameter (not shown). However, the optimal objective function values are considerably influenced by the smoothing parameter (see Figure 8).

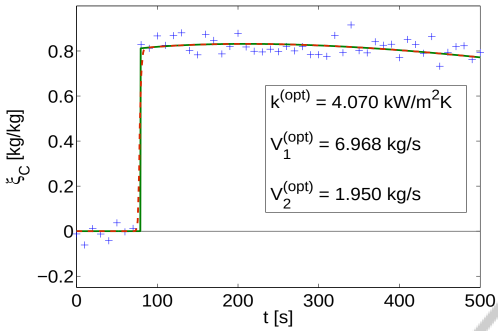


Figure 7: Parameter estimation result (dashed), measurement (cross) and simulation of the hybrid model (solid).

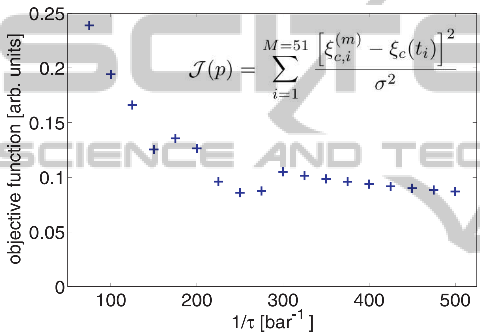


Figure 8: Optimal objective function values as a function of the smoothing parameter.

6 CONCLUSIONS

In this study, we carried out the parameter estimation accompanied by sensitivity analysis for a hybrid evaporating system using a smoothing approach. We first investigated a smooth approximated model by means of simulation of the evaporator dynamics for different values of the smoothing parameter. Performing the sensitivity analysis with respect to the parameters to be estimated we could evaluate the usability of the measurement of a certain variable for the parameter estimation. The sensitivity with respect to the smoothing parameter is studied to evaluate the suitability of the smooth model for the purpose of parameter estimation. It is shown the proposed method can successfully determine the correct parameter values. The results turned out to be quite robust against the variation of the smoothing parameter. Future work will extend the model for control tasks and finally optimize the plant operations.

REFERENCES

Barton, P. I. and Lee, C. K. (2002). Modeling, simulation, sensitivity analysis, and optimization of hybrid systems. *ACMT. Model. Comp. S.*, 12(4):256–289.

Barton, P. I., Lee, C. K., and Yunt, M. (2006). Optimization of hybrid systems. *Comp. Chem. Eng.*, 30(10-12):1576–1589.

Baumrucker, B. T., Renfro, J. G., and Biegler, L. T. (2008). MPEC problem formulations and solution strategies with chemical engineering applications. *Comp. Chem. Eng.*, 32(12):2903–2913.

Goebel, R., Sanfelice, R. G., and Teel, A. R. (2009). Hybrid dynamical systems. *IEEE Control Syst. Mag.*, pages 28–93.

Mehrmann, V. and Wunderlich, L. (2009). Hybrid systems of differential-algebraic equations - analysis and numerical solution. *J. Process Contr.*, 19(8):1218–1228.

Pappala, V. S. and Erlich, I. (2008). A new approach for solving the unit commitment problem by adaptive particle swarm optimization. In *Power and Energy Society General Meeting, 2008 IEEE*, pages 1–6.

Prada, C. D., Cristea, S., and Rosano, J. J. (2007). Optimal start-up of an evaporation station. In *8th International IFAC Symposium on Dynamics and Control of Process Systems*, volume 3, pages 115–120.

Ralph, D. and Wright, S. J. (2004). Some properties of regularization and penalization schemes for MPECs. *Optim. Method. Softw.*, 19(5):527–556.

Sager, S. (2009). Reformulations and algorithms for the optimization of switching decisions in nonlinear optimal control. *J. Process Contr.*, 19(8):1238–1247.

Sonntag, C., Stursberg, O., and Engell, S. (2006). Dynamic optimization of an industrial evaporator using graph search with embedded nonlinear programming. In *2nd IFAC Conference on Analysis and Design of Hybrid Systems*, pages 211–216.

Sonntag, C. and Stursberg, O. (2005). Safety verification of a discretely controlled evaporation system. In *Technical Report, HYCON*, pages 1–20.

Till, J., Engell, S., Panek, S., and Stursberg, O. (2004). Applied hybrid system optimization: An empirical investigation of complexity. *Control Eng. Pract.*, 12:1291–1303.

Voelker, A., Sonntag, C., Lohmann, S., and Engell, S. (2007). Optimization-based safety analysis of an industrial-scale evaporation system with hybrid dynamics. In *8th International IFAC Symposium on Dynamics and Control of Process Systems*, volume 1, pages 117–122.