

**DYNAMIC OPTIMIZATION OF AN
INDUSTRIAL EVAPORATOR USING GRAPH
SEARCH WITH EMBEDDED NONLINEAR
PROGRAMMING**

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Abstract: In this paper, we consider the task to start the operation of an industrial evaporation system. Rigorous modelling gives rise to a hybrid automaton with large nonlinear DAE-models that describe the continuous evolution in the discrete locations. The optimization problem is solved by a hierarchical procedure that consists of a branch-and-bound algorithm with embedded nonlinear dynamic optimization over a finite look-ahead horizon. Important elements of the algorithm are the introduction of a dynamic choice of the time intervals over which the controls are constant and of tailored penalty functions in order to obtain solutions which are close to infeasible trajectories. *Copyright © 2006 IFAC*

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1. INTRODUCTION

Chemical processing systems usually exhibit nonlinear and, in case of changes of the physical state of the substances (e.g. from liquid to vapour), switched dynamics. In addition, the states and the inputs are constrained, and a considerable number of actuated inputs usually is of discrete nature, e.g. valves which can be either open or closed. Besides continuous feedback controllers, there are logic (switching) controls that establish sequential procedures and initiate exception routines if malfunctions of sensors or actuators or serious disturbances occur. An important function of logic

controls is for example the safe shut-down of the plant in case of dangerous situations. In order to describe such automated processing plants, hybrid models with nonlinear dynamics are appropriate. However, the computation of optimal controls for such models is very challenging due to the usually large number of discrete degrees of freedom in connection with the nonlinear dynamics. As an example, the hybrid model of a simplified industrial evaporation system is described in this paper, and the task of optimal start-up of this plant is formulated. The evaporator is a simplified version of a benchmark example that was developed within the EU Network of Excellence HYCON in cooperation with an industrial partner.

Due to the complexity of the hybrid model, the application of techniques which evaluate the optimality conditions, see e.g. (Sussmann, 1999; Bran-

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location $z \in Z$. For given input trajectories $u(t)$ and $v(t)$ and a location $z \in Z$, we assume that a unique solution of $M\dot{x}(t) = f(z, x(t), u(t), v(t))$ exists for an initialization $x(0) \in \text{inv}(z)$, $t \in \mathbb{R}^{\geq 0}$, and $M \in \mathbb{R}^{n \times n}$, $M_{ij} = 0 \forall i \neq j$; $i, j \in \{1, \dots, n\}$; note that f constitutes a system of semi-explicit differential-algebraic equations (DAEs) if M is not regular;

- and the *output function* $l : X \rightarrow Y$ which uniquely maps the evaluation of the continuous variables to output variables $y(t) \in Y$. \diamond

Let $\Sigma = \bigcup_{z \in Z} \bigcup_{x \in \text{inv}(z)} (z, x)$ denote the set of valid *hybrid states* $\sigma = (z, x)$ of *HA* with $z \in Z$, $x \in \text{inv}(z)$. $T = \{t_0, t_1, t_2, \dots\}$ is the ordered set of time points $t_k \in \mathbb{R}^{\geq 0}$ which contains the initial time $t_0 = 0$ and all points of time at which an input changes or a transition occurs. For $t_k \in T$, the hybrid states, inputs, and outputs are written as: $\sigma_k := (z_k, x_k)$, $u_k := u(t_k)$, $v_k := v(t_k)$ with $(u_k, v_k) \in \psi(z_k)$, and $y_k := y(t_k)$.

A continuous input trajectory defined on T is a sequence $\phi_u = (u_0, u_1, u_2, \dots)$, and a discrete input trajectory is given by $\phi_v = (v_0, v_1, v_2, \dots)$, meaning that u_k and v_k are piecewise constant on $[t_k, t_{k+1}[$. For given ϕ_u and ϕ_v , a sequence $\phi_\sigma = (\sigma_0, \sigma_1, \sigma_2, \dots)$ of hybrid states $\sigma_k = \sigma(t_k) = (z_k, x_k)$ is a deterministic *feasible run* of *HA* iff:

- $\sigma_0 = (z_0, x_0)$, with $x_0 \in \text{inv}(z_0)$, and
- $\sigma_{i+1} = (z_{i+1}, x_{i+1}) \in \Sigma$ follows from $\sigma_i = (z_i, x_i) \in \Sigma$ according to:
 - $\bar{x}_{i+1} = x(t_{i+1})$ is the continuous state obtained from solving $M\dot{x}(t) = f(z_i, x(t), u(t), v(t))$ for $t \in [t_i, t_{i+1}[$ starting from $x_i = x(t_i)$, and $x(t) \in \text{inv}(z_i)$ must apply for all $t \in [t_i, t_{i+1}[$, and $x(t) \notin g(\theta)$ for $t \in [t_i, t_{i+1}[$ and for all $\theta = (z_i, \bullet)$.
 - if $\bar{x}_{i+1} \in g(\theta)$, $\theta = (z_i, z')$: $z_{i+1} := z'$, $x_{i+1} := j(\theta, \bar{x}_{i+1}) \in \text{inv}(z_{i+1})$;
 - else $x_{i+1} := \bar{x}_{i+1}$, $z_{i+1} := z_i$. \diamond

2.2 HA Model for the Evaporator

Since product can be drained from the vessel only if the target region (see Sec. 3) is reached, it is sufficient to introduce four locations, i.e. $Z = \{z_{NE}, z_{NET}, z_E, z_{ET}\}$, where 'E' stands for evaporating, 'NE' for not evaporating, and 'T' for target. The continuous dynamics of all locations is modeled by a DAE system with four differential equations (modeling the the total masses of the three components m_1 (product), m_2 (water), and m_3 (alcohol), and the total inner energy U), and 13 algebraic equations that were derived using the assumption that the system is in thermodynamical equilibrium during evaporation. The algebraic variables are the mass fractions of the three components in the liquid phase (w_1, w_2, w_3) and in the vapor phase (ξ_1, ξ_2, ξ_3), the temperature in the

evaporator T , the total mass of the liquid m_{liq} , the volume of the vapor phase V_{vap} , the energy transfer between the heat exchanger and the evaporator \dot{Q} , the mean temperature T_m and the pressure P_{HE} in the heat exchanger, and the flow rate of hot steam into the heat exchanger \dot{F}_{HE} . If the system is in location z_{NE} , the variables ξ_1, ξ_2, ξ_3 , and V_{vap} are set to zero since a vapor phase does not exist. As an example for the high degree of complexity and nonlinearity of the DAE-system, the equation describing the equilibrium conditions for the mass of the alcoholic component looks like:

$$m_3 = m_{liq} \cdot w_3 + \frac{w_3 \cdot P_3^0(T) \cdot V_{vap}}{R \cdot T \cdot \left[\frac{w_1}{M_1} + \frac{w_2}{M_2} + \frac{w_3}{M_3} \right]} \quad (1)$$

with the universal gas constant R , the molecular weights M_1, M_2 , and M_3 , and $P_3^0(T)$ is a third-order polynomial in T .

Using the justifiable assumption that the liquid mass m_{liq} and the mass fractions w_1, w_2 , and w_3 remain constant for any transition θ , all hybrid states $\sigma = (z, x)$ of the evaporator are uniquely determined by a reduced vector:

$$x_{red} = [w_1, w_2, T, L, P]. \quad (2)$$

The output variables L and P , which can be uniquely determined from the state variables, represent the liquid level and the pressure in the evaporator². While L follows from the mass and density of the liquid, P is given by:

$$P = \frac{\frac{w_1}{M_1} \cdot P_1^0(T) + \frac{w_2}{M_2} \cdot P_2^0(T) + \frac{w_3}{M_3} \cdot P_3^0(T)}{\frac{w_1}{M_1} + \frac{w_2}{M_2} + \frac{w_3}{M_3}}, \quad (3)$$

where $P_1^0(T)$, $P_2^0(T)$, and $P_3^0(T)$ are third-order polynomials in T .

A bounded and reduced continuous state space can be defined as:

$$X_{red} = [0, 0.98] \times [0, 1] \times [300, 440] \times [0, 100] \times [0, 5], \quad (4)$$

and $x_{red} \in X_{red}$. (Units are omitted for abbreviation.) During start-up, the upper bounds given in Eq. 4 must not be exceeded for safety reasons.

The continuous inputs u_1 and u_2 represent the settings of the valves V_{V1} and V_1 , and are defined on the range $[0 \%, 100 \%]$, where 0 % means completely closed. For all $z \in Z$, both continuous inputs are available. A discrete input is defined as the vector $v_j = (V_2, V_{V2})$ and the discrete input space by $V = \{(0 \%, 80 \%), (0 \%, 100 \%), (11.5 \%, 80 \%), (11.5 \%, 100 \%)\}$. If $z \in \{z_{NE}, z_E\}$, the product drain valve must remain closed, such

² The dynamics of the process is nevertheless determined by the higher-order DAE-system since the latter cannot be solved explicitly for x_{red} , i.e. the use of x_{red} does not reduce the model complexity.

that the available discrete inputs are reduced to $\mathcal{V}_{z_{NE}, z_E} = \{(0\%, 80\%), (0\%, 100\%)\}$. Otherwise, all discrete inputs are available.

Between all pairs of locations, transitions in both directions can occur, i.e. $|\Theta| = 12$. The transitions can be divided into three classes: (a) transitions occurring if the product concentration reaches or leaves the target region (see Sec. 3), (b) transitions occurring when the liquid begins or stops to evaporate, and (c) transitions for which both is true. While the guard condition for (a) only depends on the current value of w_1 , the guard set for (b) is assumed to be given by $P = 0.4$, with P defined according to Eq. 3. The guard for (c) is the conjunction of the two previous ones. The invariants of the locations are bounded by the set of states defined by the guard conditions and the boundaries in Eq. 4. Although the state variables ξ_1, ξ_2, ξ_3 , and V_{vap} are reset with discrete transitions of the hybrid model, the variables in x_{red} are not affected due to the modeling assumptions described above.

3. THE OPTIMAL CONTROL PROBLEM

The following type of optimal control problem is considered in this paper: Given are an initial state $\sigma_0 \in \Sigma$ and a target set $\Sigma_t \subset \Sigma$ with $\Sigma_t = \{(z_t, x) | \exists_1 z_t \in Z : x \in X_t \subset \text{inv}(z_t)\}$. It is assumed that the ordered set of time points $T = \{t_0, t_1, t_2, \dots, t_f\}$ is finite, and that the continuous and discrete inputs can only be changed at $t_k \in T_s \subset T$, while ϕ_σ remains defined on T . The set $\Phi_{u,s}$ contains all possible continuous input trajectories $\phi_u = (u_0, u_1, u_2, \dots)$ defined on T_s , and $\Phi_{v,s}$ contains all possible $\phi_v = (v_0, v_1, v_2, \dots)$. The control task is then to determine input trajectories ϕ_u^* and ϕ_v^* that lead to a feasible run ϕ_σ^* of HA from σ_0 into Σ_t such that a cost function Ω is minimized:

$$\begin{aligned} \min_{\phi_u \in \Phi_{u,s}, \phi_v \in \Phi_{v,s}} \quad & \Omega(t_f, \phi_\sigma) \\ \text{s.t.} \quad & \phi_\sigma = (\sigma_0, \dots, \sigma_f) \text{ with } \sigma_0 = (z_0, x_0), \\ & \sigma_f := (z(t_f), x(t_f)) \in \Sigma_t. \end{aligned} \quad (5)$$

The initial state of the evaporator is given by $x_{0,red} = [0.12, 0.85, 327, 1, 0.282]$, denoting a state with very low product concentration, low level, and no evaporation ($z_0 := z_{NE}$). The control task is to drive the system into the location $z_t = z_{ET}$ and the target region $X_{t,red} = [0.8, 0.84] \times [0.16, 0.2] \times [370, 420] \times [60, 64] \times [0.5, 4]$ in a time-optimal fashion.

Using the cost function $\Omega = t_f$ in (5) and optimizing over the complete time horizon $[t_0, t_f]$ is often computationally intractable since $|T_s|$ choices for u and v lead to an exponential growth of the solution space with increasing $|T_s|$. In this case,

a substitute for Ω may be chosen which allows for an appropriate cost evaluation of trajectories also over shorter time horizons. A possible choice is a cost function which combines t_f with a notion of distance of any intermediate state σ_k to the target region Σ_t . It was found for the evaporator, however, that this choice for Ω does provide only solutions for which t_f is somewhat worse than the optimal value. Reasoning about the expected behavior of the system led to the following heuristically-chosen cost function:

$$\Omega(x_{s,red}) = \begin{cases} \alpha \cdot |w_{s,1} - w_{s,1,t}| + \beta \cdot |L_s - L_{s,max}| & \text{if } |w_{s,1} - w_{s,1,t}| > 0.09, \\ \beta \cdot |w_{s,1} - w_{s,1,t}| + \alpha \cdot |L_s - L_{s,t}| & \text{if } |w_{s,1} - w_{s,1,t}| \leq 0.09. \end{cases} \quad (6)$$

Note that before evaluating $\Omega(x_{s,red})$, all variables of x_{red} are scaled to the range $[0, 1]$ according to $x_{s,red} = D^{-1} \cdot x_{red} - c$, with $D = \text{diag}(0.98, 1, 140, 100, 5)$ and $c = [0, 0, 2.1429, 0, 0]^T$. In Eq. 6, $w_{s,1}$ is the scaled product concentration, $w_{s,1,t} = 0.804$ the scaled target concentration, L_s the scaled liquid level, $L_{s,max} = 1$ the upper bound for L_s , $L_{s,t} = 0.62$ is the scaled target level, and α and β denote weighting constants. The motivation for this choice of $\Omega(x_{s,red})$ is that the fastest way to increase $w_{s,1}$ should be to maximize the energy transfer \dot{Q} between the heat exchanger and the evaporation vessel (and thus, the evaporation rate of the volatile components). The energy transfer increases with the difference between the liquid temperature T and the temperature of the hot steam. If the liquid level L is held close to its maximum value, a minimal temperature of the liquid is achieved. After the product concentration has reached a threshold which is close to its target value, the level has to be driven into the target region. In order to push the increase of $w_{s,1}$ which exhibits slow dynamics, the constant weights were chosen according to $\frac{\alpha}{\beta} = 4$ if $|w_{s,1} - w_{s,1,t}| > 0.09$. For $|w_{s,1} - w_{s,1,t}| \leq 0.09$, the weights were chosen according to $\frac{\beta}{\alpha} = 4$ to put the focus on driving L_s into the target.

4. THE OPTIMIZATION APPROACH

The approach used here for optimizing the start-up of the evaporator is based on the graph search algorithm presented in (Stursberg, 2004a; Stursberg, 2004b). This section first reviews the basic principle, and then describes necessary modifications to solve the case study.

4.1 Graph Search with Embedded NLP

The main idea of the approach is to separate the optimization of the discrete and continuous degrees of freedom by encoding the discrete choices

vapor drain through V_{V1} is maximized while L is held at 100 % using appropriate settings for V_1 . Towards the end, V_1 is closed to drive the liquid level into the target region. V_2 is always closed since w_1 is the last variable to reach the target region, and V_{V2} remains open. During the optimization, 600 nodes were investigated, and 96 solutions were found. The complete optimization run took around 6 hours on a PC with Pentium-IV 2.8 GHz. The best solution was determined after 746 seconds, and using the input trajectories defined by this solution, the target region is reached after 13937 seconds.

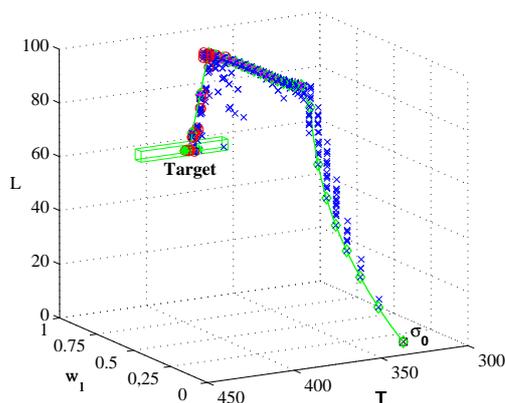


Fig. 3. Explored nodes and the state trajectory of the best solution.

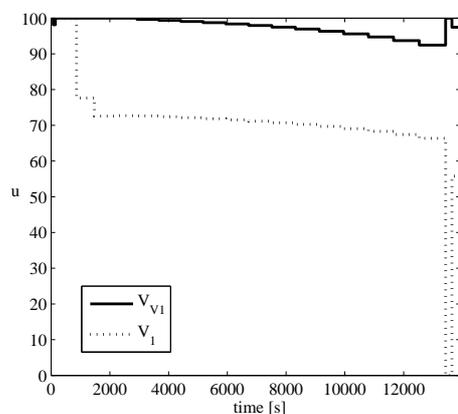


Fig. 4. Continuous input trajectories for the best solution.

6. CONCLUSIONS

The problem of optimizing the start-up of a hybrid model of an industrial-scale evaporator with complex nonlinear continuous dynamics was tackled using a graph search algorithm with embedded nonlinear programming. To obtain feasible and good solutions with the algorithm, two modifications had to be introduced: (a) a state-dependent

termination criterion for the embedded hybrid simulation, and (b) a modified cost function for the NLP step to rule out infeasible evolutions while allowing optimization near or on the boundary of invariants.

The next steps of this research are as follows: We try to develop schemes that are able to find feasible solutions for similarly challenging problems without the requirement of first determining specifically tuned cost functions (as described in Sec. 3). In addition, we aim at extending the solution concept presented here to the multi-stage evaporator as described in (Sonntag and Stursberg, 2005).

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