Maximal safe set computation for pressure swing adsorption processes

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A B S T R A C T

In this paper we propose a method towards purity control of pressure swing adsorption (PSA) processes which is based on the use of hybrid systems formalism. Hybrid systems feature both continuous and discrete-event dynamics and hence are very suited to describe in detail PSA processes. Based on mechanistic model of the processes, a local reduced-order model (LROM) is developed for PSA processes. Then the processes are represented as hybrid systems whose continuous evolution is described by the LROM. We then perform an analysis of hybrid reachability properties of the hybrid system obtained, based on which the so-called maximal safe set is computed. The analysis is performed for a two-bed, six-step benchmark PSA process and the influence of the control inputs and external disturbances are investigated.

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1. Introduction

Pressure swing adsorption (PSA) plants are well-known and are widely used for separation and purification of gas mixtures. In PSA processes, cyclic and selective adsorption/desorption of gas species at higher/lower pressures results in separation of gas components. Industrial PSA plants consist of several interconnected adsorption beds from 2 to 20 beds (Ruthven et al., 1994; Elseviers et al., 2015). The flow rates and directions of the gas streams between the adsorption beds are controlled by a network of interconnecting valves whose status changes from one process mode to the next. Each adsorption bed is a distributed parameter system that can be described by a set of partial differential algebraic equations (PDAEs) with changing boundary conditions, which are forced by the status of the control valves corresponding to different modes of the process. During each mode of the process, the arrangement of the valve network is fixed and the adsorption beds are in specific cycle-steps. The transition time of the process modes is determined by timed or controlled discrete-events. Accordingly, PSA processes are finite dimensional hybrid systems (Branicky et al., 1998; Rivotti and Pistikopoulos, 2015; Lygeros et al., 1999) with known and fixed mode sequences in which their continuous dynamics is influenced by the cyclic mode transition events.

Recently, the control of PSA processes attracted much interest, although very few studies were reported in the open literature (Bitzer, 2005; Torre et al., 2005; Mulholland and Latifi, 2009; Khajuria and Pistikopoulos, 2013; Sun et al., 2015) which are focused on regulation of switch times of PSA systems mainly based on estimated/measured product purity of the process. Bitzer and Zeitz (2002) and Bitzer (2005) presented a purity control scheme consisting of a model-based feedforward and a linear feedback controller. The feedforward controller was set up by an inverse reduced-order model (ROM) based on empirical wave functions that are approximating the concentration profiles of the gas species along the adsorption beds. The controller proposed was verified in a two-bed, four-step PSA system producing oxygen from air. Torre et al. (2005) proposed a model predictive control (MPC) for purity control of a single-bed, six-step vacuum swing adsorption (VSA) process used for oxygen production from air. An approximated linear input–output (I/O) model was used for a single-input-single-output (SISO) MPC controller, Mulholland and Latifi (2009) used a predictive controller based on a linearized model for set-point
tracking control of a single adsorption bed for air separation, and solved a mixed integer dynamic optimization. Khajuria and Pistikopoulos (2011, 2013) proposed an explicit/multi-parametric MPC design framework applied to PSA systems, based on an approximated SISO linear I/O model of the PSA processes. The controller was designed for H2 purification from a H2–CH4 gas mixture in two case studies of four-bed, nine-step and two-bed, six-step PSA processes. Sun et al. (2015) used a regulatory proportional-integral-derivative (PID) controller in a PVSA process for CH4 recovery from a N2–CH4 gas mixture.

Synthesizing a hybrid controller (Lygeros et al., 1999) with respect to the hybrid nature of the PSA processes (Fakhrholeslami et al., 2017) was not considered in the aforementioned studies. A hybrid controller is composed of an event-driven part and a continuous part which regulate the controllable event-driven and continuous inputs, respectively. In this work, in order to design a hybrid controller for PSA processes, computation of maximal safe set by means of hybrid reachability analysis (Asarin et al., 2006; Bayen et al., 2007) is investigated for PSA processes. The reachable set of a hybrid system, the computation of which is often motivated by safety verification (Sonntag et al., 2008), consists of all the hybrid states that can be reached by a trajectory of the hybrid system starting in a specified set of initial states. The maximal safe set is defined as the set of all hybrid states from which there exists a control strategy that can maintain the system inside a specified safe region forever, even in the presence of external disturbances. The performance of the PSA processes is usually determined by their product purity along with product recovery and process productivity. However, the main control objective is to maintain the product purity at a specific purity set-point despite the action of external disturbances like flow rate, composition, and temperature of the feed stream. The available control actions are the mode transitions and purge-to-feed ratio (PFR). This control objective is represented as a safety problem (Sonntag et al., 2008) for PSA processes in which the purity must be higher than a specific threshold. The defined safety problem is solved based on hybrid reachability analysis.

Computation of the maximal safe set can be represented as a two-player game between the controller and the open-loop behavior of the plant under external disturbances. The controller as Player I wants to maintain the plant in a safe region while the plant and external disturbances as Player II force the system into unsafe. A procedure for such computation in case of a hybrid system is developed by Tomlin et al. (1998, 2000). The safety specifications of the hybrid system were translated into restrictions on the system’s reachable sets of states. Then, by analysis based on two-player zero-sum game theory for autormata (Barton et al., 2006; Lygeros et al., 2012) and continuous dynamical systems, the Hamilton–Jacobi–Isaacs (HJI) partial differential equations (PDEs) whose viscosity solutions describe an implicit surface representation of the backward reachable unsafe set, were derived.

The level set method (Osher and Fedkiw, 2002) is employed in computation of the backward reachable sets which are described as a dynamic implicit surface. An implicit surface defines a function \( \phi \) as a possible level set function describing a set of states \( G \) such that \( \phi < 0 \) if the states are inside \( G \), \( \phi = 0 \) if the states are on the boundaries of \( G \), and \( \phi > 0 \) if the states are outside \( G \). A schematic of a level set function (surface) and its zero-level set (curve) is illustrated in Fig. 1. The level set methods have been developed and well studied for numerical solution of time-dependent HJ PDEs and the propagation of moving interfaces and boundaries. Implementation of numerical solution of HJI PDE by means of level set methods is well explained by Osher and Fedkiw (2002) and Mitchell et al. (2005).

In practice, solutions to the HJI PDE are computationally expensive and have been shown to be efficient in two- or three-dimensions, although scalable reachability analysis for systems with nonlinear dynamics is still an open problem in control and computer science (Chen et al., 2016; Akametalu and Tomlin, 2015). Accordingly, in order to implement such a solution method and controller design in the case of distributed parameter hybrid systems with huge number of continuous states, like PSA, development of a minimal ROM is unavoidable. ROMs are low-dimensional efficient models that provide fast and high-fidelity approximation of the system behavior. The field of reduced-order modeling encompasses a broad set of mathematical methods to generate and
evaluate ROMs, and new techniques are developing rapidly. Interested readers can obtain an overview of the recent works on ROMs in (Antoulas, 2005; Benner et al., 2015; Beattie et al., 2017) and references therein. The use of ROMs for simulation, optimization, and control of the PSA processes, which are described by a set of PDAEs, is inescapable. Almost all of the reported works in this area, e.g. (Malek and Farooq, 1997; Ribeiro et al., 2008; Agarwal et al., 2008; Khajuria and Pistikopoulos, 2011; Fakhroleslam et al., 2016), use reduced-order models to convert the PDAE model to an ordinary differential algebraic equation (ODAE) model which can be solved by standard ODE solvers. Bitzer and Zeitz (2002) and Bitzer (2005) developed a ROM for PSA process based on several empirical wave functions to obtain the dynamics of all process variables. Torre et al. (2005) and Khajuria and Pistikopoulos (2011) used linear SISO PSA models as ROMs that are approximated by data-driven model identification techniques. In this work, a local ROM (LROM) is developed for approximation of the dynamical behavior of PSA processes at a specific location of its adsorption beds. The operational constraints, external disturbances, and available control actions of the process are also incorporated in the LROM. Then the process model is formalized as a hybrid system whose continuous and discrete-event behaviors are described by the LROM and an automata, respectively. Based on the obtained hybrid model, the hybrid reachability analysis is feasible.

The rest of the paper is organized as follows. In Section 2, a mechanistic mathematical model is presented for PSA processes and as a case study, a two-bed, six-step PSA process for H2 purification from a H2–CH4 gas mixture is introduced. Then a LROM is developed based on the full-order model. The process model is described as a hybrid system in Section 3. Then in Section 4 the purity control problem is formalized as a safety problem for hybrid systems and the procedure for computation of the maximal safe set is explained. The results are reported and discussed in Section 5, and finally the paper is concluded in Section 6.

2. PSA process

As a case study, consider the two-bed, six-step PSA system, illustrated in Fig. 2 along with the corresponding scheduling table for arrangement of the solenoid valves in the switching modes of the process. The adsorption beds contain activated carbon as adsorbent used for separation of a H2–CH4 gas mixture. The objective is to obtain a high purity H2 product from a H2–CH4 mixture whose H2 mole fraction is 70%. The structure of the PSA system and the sequence of the operating steps are fixed. Each cycle of the considered PSA process consists of six sequential steps including adsorption (ADS), depressurization equalization (DPE), blow down (BDN), purge with product (PRG), pressurization equalization (PEQ), and re-pressurization (REP). For instance in mode q4, valves V-02, V-03, V-05, and V-08 are open and subsequently BED1 undergoes PRG while BED2 is in ADS step.

The main control objective in PSA processes is to adjust the purity to be at a specific set-point and higher than a threshold according to requirements of a specific application. The product is produced during the ADS step of an adsorption bed, hence, the product purity is available during modes q1 and q4. When BED1 and BED2 are in their ADS step during q1 and q4, respectively. As it can be seen in the scheduling table in Fig. 2, BED1 and BED2 are in their ADS step during q1 and q4, respectively. The purity specification has to be satisfied in the presence of various noise and external disturbances. Two disturbances that have the most significant effects on the performance of PSA processes are the variations of flow rate and mole fraction of the feed stream that are forced to PSA processes from upstream units. The flow rate Qf and the CH4 mole fraction y0 of the Feed stream, are considered as continuous disturbances which can vary in ±25% and ±8% intervals around their nominal values, Qf0 and y0, respectively, i.e. \( \frac{Qf}{Qf0} \in [0.75, 1.25] \) and \( \frac{y0}{y0} \in [0.92, 1.08] \). Mode transition and

![Fig. 1. (a) A level set function \( \phi(x_1, x_2) \) and (b) its zero-level set \( \phi(x_1, x_2) = 0 \); the level set function \( \phi \) shown in (a) is a possible implicit function for the two-dimensional domain in (b) that defines the domain’s boundary \( \phi = 0 \), inside portion \( \phi < 0 \), and outside portion \( \phi > 0 \).](image1)

![Fig. 2. Schematic of a two-bed, six-step PSA plant and the corresponding scheduling table for arrangement of the solenoid valves in the switching modes of the process.](image2)
PFR are two available control inputs. The former is an event that switches the active mode of the process by changing the arrangement of the interconnecting valves, and the later is the ratio of the flow rate of purging stream (adjusted by MFC1 in Fig. 2) to that of the feed stream (measured by MFM1). The PFR, denoted by rp, is considered to be ranged in a ±15% interval around its nominal value, i.e., $\frac{rp}{rp_{n}} \in [0.85, 1.15]$. Therefore, the process has two continuous disturbances, and two control actions: one discrete and one continuous. The control inputs have to be designed so that the efficient performance of the process is guaranteed under the action of the external disturbances.

From the process knowledge and numerical simulations of the benchmark PSA process, it is known that approximately $\bar{t} = 12.1$ s is required for pressure transitions during the modes $q_{2}$, $q3$, $q5$, and $q6$. On the other hand, the nominal value of switching times ($t_{gp}$) for modes $q_{1}$ and $q_{4}$ corresponds to the purity-set point which should be obtained at a normal cyclic steady state (CSS) condition (in the absence of the external disturbances).

2.1. Nonlinear non-isothermal model for adsorption beds

The mathematical model of adsorption beds can be obtained based on the total and component mass balances in gas and solid phases, along with the energy balance, adsorption equilibrium isotherm model, and pressure drop equations. It is assumed that the ideal gas law is acceptable for the gas mixture over all operating ranges of pressure and temperature. The radial variations of concentration and temperature inside the adsorption beds are neglected and the flow pattern is described by the axially dispersed plug flow. It is assumed that the beds are uniformly packed with fixed spherical solid adsorbents. The bed including the solid–gas system and the bed’s wall are assumed to be in thermal equilibrium (Khajuria and Pistikopoulos, 2011) and the adsorption beds are well-insulated. The axial mass and heat transfer dispersion coefficients, i.e., $D_{m}$ and $\lambda$, are assumed to be constant and does not depend on the velocity (Wakao and Funakazi, 1978; Wakao et al., 1979). The axial velocity–pressure equation inside the bed is obtained by steady state Ergun equation (Biegler et al., 2005) and the intra-particle mass balance is described by linear driving force (LDF) model (Ruthven et al., 1994). The main equations and the boundary conditions of the model are listed in Tables 1 and 2. The dynamics of the process inside the adsorption beds can be obtained by the set of PDAEs given in Table 1. The state variables inside the adsorption beds are affected by the time-varying boundary conditions at the bottom and top of the beds in different modes of the process. The continuous disturbances and control inputs can also be incorporated in the model by making variations in boundary conditions of the adsorption beds. The feed composition in ADS step can be changed directly, and the superficial velocities in ADS and PRG steps are related to $Q_{i}$ and $r_{gp}$ as $v_{i} = \frac{Q_{i}}{A_{gp}}$, and $v_{pde} = r_{gp} \times v_{i}$. The detailed description of the first-principle based model along with the model parameters are available in the previous works by Fakhruleslam and Fatemi (2016) and Fakhruleslam et al. (2016) and the references therein.

Regarding the 1st gas component as the main gas component to be separated, the product purity $Pur^{S}$ and recovery $Rec^{S}$ of the $\theta$th adsorption bed of a PSA process are defined by Eqs. (1) and (2), respectively:

$$Pur^{S} = \frac{\int_{t_{0}}^{t_{f}} (C_{1}(t)\nu(t))^{S}_{ze} dt}{\sum_{i=1}^{N_{ads}} \int_{t_{0}}^{t_{f}} (C_{i}(t))^{S}_{ze} dt}$$

$$Rec^{S} = \frac{\int_{t_{0}}^{t_{f}} (C_{1}(t)\nu(t))^{S}_{2e} dt - \int_{t_{0}}^{t_{f}} (C_{1}(t)\nu(t))^{S}_{2d} dt}{\int_{t_{0}}^{t_{f}} (C_{1}(t)\nu(t))^{S}_{2e} dt}$$

where the times $t_{0}$ and $t_{f}$ with $s = \{ads, pde, rep\}$ denote the current times respectively at the beginning and at the end of the ADS, PRG, and REP steps.

2.2. A local reduced-order model for PSA process

With respect to the requirements of the hybrid reachability analysis, a LROM is proposed based on the full-order model of the process to describe the dynamical behavior of PSA processes at a specific location $z = al$, $a \in [0, 1]$ of its adsorption beds.

The adsorption isotherm model, which describes the maximum possible adsorption capacity of the adsorbent particles, is the heart of the PSA model and the source of nonlinearity and transitions of the whole process. The loaded value of the ith gas component, $Q_{i}$, is...
is the state variable that can describe the transitional behavior of the process. Accordingly, $\dot{Q}_i$ is considered as the variable based on which the controller can make appropriate decisions. By using of the proposed LROM, one can obtain the dynamics of the loading values of the gas components $\dot{Q}_i$ at the location $z=aL$ of the $i$th adsorption bed, denoted by $\dot{Q}^{al}_i$. Where $a$ is a design parameter to be specified by an expert based on the process knowledge and simulation profiles. From now on, for notational simplicity, $\dot{Q}^{al}_i$ is denoted by $\dot{Q}_i$. The parameter $a$ should be selected with respect to the control objectives, e.g. product purity and recovery, which are defined at the end of the adsorption beds where $z=L$. The idea behind this is the well-known fact that the state variables along the adsorption beds of a PSA process can be described by traveling waves through the beds and there are strong interconnections between them.

In order to simplify the process model to obtain the LROM, the following assumptions are placed. The process is assumed to be isothermal in which the temperature is constant along the adsorption bed throughout the time. Pressure drop along the adsorption bed's length is ignored and it is assumed that the spatial pressure profile is uniform along the bed, although the spatially uniform profile is time-varying in the cycle-steps with pressure transition. The total concentration is assumed to have a spatially uniform profile along the bed, which leads to a constant velocity $v$ along the adsorption bed. It is clear that all the mentioned uniform profiles are variable over time. To mimic the isothermal model of the full-order model, any arbitrary isothermal model describing pressure, thermal, and thermodynamical effects and interactions can be employed. Here, in order to show the effectiveness of the LROM, the very simple single-site Langmuir isotherm model is used for description of the adsorption equilibrium.

The dynamics of $P^{al}_i$ and $\dot{Q}^{al}_i$ for the $i$th adsorption bed are given, respectively, by:

$$\dot{P}^{al}_i(t) = f(P^{al}_i(t), q)$$

(3)

$$\dot{Q}^{al}_i = \frac{K_{LDF}(Q^{al}_i(t), P^{al}_i(t), q)}{1 + \frac{q}{b_i y_i q(Q^{al}_i(t))}}$$

(4)

where, by assuming that the competitive effect of different components is negligible, the maximum possible adsorption capacity can be approximated by the single-component Langmuir isotherm model as:

$$Q^{al}_i(P, \Delta, u, q) = \frac{a_i y_i q(Q^{al}_i) + \Delta y_i}{1 + b_i y_i q(Q^{al}_i)}$$

(5)

with $a_i$ and $b_i$ constant parameters of the isotherm equation, where $y_i q$ is mole fraction of the $i$th component at $z=aL$ that can be described by an arbitrary equation whose coefficients are adapted based on numerical simulations by the full-order model. Eq. (5) is valid around the CSS in the absence of any control inputs and external disturbances, and in case which the competitive effect of different components is negligible. In this work a linear relationship between $y_i q$ and $\dot{Q}_i$ in each mode $q$ is considered as:

$$y_i q(Q^{al}_i) = a_{iq} Q^{al}_i + b_{iq}$$

The parameters $a_{iq}$ and $b_{iq}$ are constant in each process mode $q$. However, since the isothermal model is the most important part of the LROM, it should be selected precisely with respect to the specifications of the process and the present gas components. The dynamics of $P^{al}_i$ which is described by the function $f_{(\dot{P}^{al})}$ in Eq. (3) depends on the characteristic curve of the interconnecting valves.

The next step is to incorporate the model of control inputs and disturbances into the continuous dynamics of the proposed LROM. During adsorption step (ADS), as the flow rate of the feed stream increases with constant mole fraction, the amount of impurities that are supposed to be adsorbed, increases. The same behavior is expected as the mole fraction of impurities in feed stream increases.

### Table 3

<table>
<thead>
<tr>
<th>Cycle-step</th>
<th>$P(t)^b$</th>
<th>$y_i(\dot{Q}_i)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>ADS</td>
<td>$P(t) = 0$ and $P(0) = P_{ads}$</td>
<td>$y_{i1} = +0.2857\dot{Q}_i + 0.0512$</td>
</tr>
<tr>
<td>DPE</td>
<td>$P(t) = t\eta(P - P_{ads})^\alpha $</td>
<td>$y_{i2} = -2.3233\dot{Q}_i + 1.963$</td>
</tr>
<tr>
<td>DBN</td>
<td>$P(t) = t\eta(P - P_{ads})^\alpha $</td>
<td>$y_{i3} = -3.0069\dot{Q}_i + 2.317$</td>
</tr>
<tr>
<td>PRG</td>
<td>$P(t) = 0$ and $P(0) = P_{rg}$</td>
<td>$y_{i4} = +1.993\dot{Q}_i - 0.1813$</td>
</tr>
<tr>
<td>PEQ</td>
<td>$P(t) = t\eta(P_{eq} - P_{ad})^\alpha $</td>
<td>$y_{i5} = +1.870\dot{Q}_i - 0.2339$</td>
</tr>
<tr>
<td>REP</td>
<td>$P(t) = t\eta(P_{eq} - P_{ad})^\alpha $</td>
<td>$y_{i6} = -0.7274\dot{Q}_i + 0.6027$</td>
</tr>
</tbody>
</table>

* The $P(t)$ descriptions are constructed based on the characteristic curves of the solenoid valves (here, Peter Paul™ 22G9DGD-NB).

On the other hand in purge step (PRG), by a constant PFR, the purge flow rate increases by increasing feed flow rate, which reduces the amount of adsorbed impurities on the adsorbent particles; whereas the effect of the feed mole fraction variations on mole fraction of the purge stream is relaxed during the separation process and it is negligible assuming that the other adsorption beds are producing a well-separated product. Therefore, increasing feed flow rate increases $\dot{Q}_i$ in the bed undergoing ADS whereas decreases $\dot{Q}_i$ in a bed that is in its PRG step. As well, increasing mole fraction of impurities in feed stream increases $\dot{Q}_i$ in ADS step and it has no significant effect on those in PRG step. The control input $P(t)$ can be included by the same reasoning. The $\eta$ affects the adsorption beds only during PRG step such that increasing $\eta$ reduces the amount of the adsorbed species. Then it has negative effect on $\dot{Q}_i$ in PRG step. These inputs are modeled as multipliers to $\dot{Q}_i$ in the isothermal model of the process. The modified isotherm model (5) is given by:

$$\dot{Q}_i(P, \Delta, u, q) = \frac{a_i y_i q(Q^{al}_i) + \Delta y_i}{1 + b_i y_i q(Q^{al}_i)}$$

(6)

where $\Delta q$ denotes the continuous disturbance which is forced to process only in ADS and PRG steps in which $\Delta_{ads} = \Delta_{q1}$ and $\Delta_{prg} = \Delta_{q2}$, respectively, $\Delta_{q1}$ is the disturbances of flow rate and mole fraction of the feed stream, respectively, $\Delta_{q2}$ denotes the control input $P(t)$ that appears only in PRG step as $u = \frac{\eta P_{eq}}{P_{eq} - P_{ad}}$ and is equal to one in the other cycle-steps. The parameters $N_0$, $N_v$, and $n_v$ can be identified based on the numerical simulations of the process. It is clear that $y_i q$, which is described as a function of $Q_i$, is influenced by the control input $P(t)$ and the disturbances (Q and y) indirectly but significantly. This is due to the fact that $\dot{Q}_i$ is the nearest state variable to the source of transitions, $Q^{al}_i$, and is highly influenced by it.

Consider the two-bed, six-step PSA process discussed above. The feed stream is a binary H2–CH4 gas mixture with CH4 as the impurity that should be removed to produce a high purity H2 product. Therefore, there is only one impurity and only one state is required for each adsorption bed to obtain the local dynamics of loaded amount of impurities, i.e. $\dot{Q}_{CH4,al}$, which will be denoted by $\dot{Q}_{CH4}$.

The logical rules of the hybrid controller will be based on the amount of adsorbed impurities at $z = aL$, i.e. $\dot{Q}_{CH4}$. As mentioned before, the design parameter $a$ should be selected with respect to the characteristics of the process. We know that the CH4-loading fronts are moving along the adsorption beds like traveling waves, in which one can find a (complex) relationship between the state variables of the LROM at $z = aL$ and the product purity at $z = L$. For the case study PSA process, since the product is high purity H2, both the impurity’s loading and its variations over time, $\dot{Q}_{CH4}$ and $\dot{Q}_{CH4}$, are insignificant near the end of the bed. This leads to low sensitivity of the product purity (at $z = L$) to $\dot{Q}_{CH4}$ near the end of the bed, and subsequently leads to weak performance of the controller. On the other hand, for small values of $a$, which provide $\dot{Q}_{CH4}$ at the begin-
ning of the adsorption bed, the variations of \( \hat{Q}_2 \) can be observed during the whole process and subsequently the process operation can be approximated properly. For the \( \mathrm{H}_2 \) purification process in this work, \( \alpha \) is fixed at \( \alpha = 0.05 \).

The dynamics of \( \hat{p}_5 \) and the equations of \( y_2 \) in different cycle-steps of the process are given in Table 3. The performance of the proposed LROM in approximation of \( \hat{Q}_{2,\alpha} \) for the adsorption beds of the two-bed PSA process, is compared against the simulation results obtained by full-order model in Fig. 3. The comparison between the simulation results of the LROM and the full-order model showed a root-mean-square error (RMSE) of 0.0056 mol/kg. It should be noted that the proposed model is valid in all operating conditions of a PSA process except for start-up and shut-down transistions of the process. This issue has been revealed by comparing the results of numerical simulations of the LORM with those of the full-order model in the presence of disturbances and control inputs. The achieved RMSEs are listed in Table 4.

Regarding the pressure dynamics in Table 3, it is possible to find analytical solutions satisfying Eq. (3) that represent \( P^2(t) \) in the adsorption beds during each mode, hence we can relax the pressure ODE in Eq. (3). Subsequently the nonlinear behavior of the process at \( z = \alpha \ell \) of 8th adsorption bed can be approximated by only one ODE given by Eq. (4) and the local dynamics of the two-bed PSA process can be described by two state variables.

In order to deal with the constraints on the switching times of the process modes, we introduce a timer \( \tau_c \) for process modes in which the mode transition in the \( q \)th mode can occur only while \( \tau_c \) is between \( \tau_q \) and \( \tau_q^+ \), the lower and upper bounds on the switching times.

Therefore the state space of the LROM for the two-bed PSA process is composed of three continuous states \( x = [Q_{2,1}^2, Q_{2,2}^2, \tau_c^2] \) : two physical states \( x_1 = Q_{2,1}^2 \) and \( x_2 = Q_{2,2}^2 \) and the timer \( x_3 = \tau_c \), with the dynamics given by

\[
\dot{x}_1(t) = K_{DF} \left( \frac{a_{p} y_2(q) y_4(q_1)(t) \Delta_1 \eta_1(q_1)}{1 + b_{p} y_2(q_1) y_4(q_1) \Delta_1 \eta_1(q_1)} - x_1(t) \right),
\]

\[
\dot{x}_2(t) = K_{DF} \left( \frac{a_{p} y_2(q_2) y_4(q_2) \Delta_2 \eta_2(q_2)}{1 + b_{p} y_2(q_2) y_4(q_2) \Delta_2 \eta_2(q_2)} - x_2(t) \right),
\]

\[
\dot{x}_3(t) = 1,
\]

where \( \Delta_1 \) and \( \Delta_2 \) are continuous disturbances, \( u_{\eta_1} \) and \( u_{\eta_2} \) are continuous control inputs, and \( \varphi(q) = \varphi_0 \). In mode \( q \), \( \Delta_1 = \Delta_{\text{ads}} \) and \( \Delta_2 = \Delta_{\text{prg}} \), and vice versa for mode \( q_4 \). With \( \eta_0 = 0.11 \) and \( n_\eta = 0.09 \), the disturbances are \( \Delta_{\text{ads}} = \left( \frac{Q_0}{m_\eta^2} \right) \left( \frac{\varphi_0}{\varphi} \right)^{0.11} \) and \( \Delta_{\text{prg}} = \left( \frac{Q_0}{m_\eta^2} \right) \left( \frac{\varphi_0}{\varphi} \right)^{0.09} \). Regarding the bounds on the continuous disturbances \( Q_0 \in [0.75, 1.25] \) and \( \varphi_0 \in [0.92, 1.08] \), the belonging intervals of the modeled disturbances are \( \Delta_0 \in [0.9689, 1.0248] \) and \( \Delta_\eta \in [0.9925, 1.0070] \). About the control inputs, with \( n_\eta = 0.15 \), in mode \( q_1 \), \( u_{\eta_1} = 1 \) and \( u_{\eta_2} = \left( \frac{\varphi_0}{\varphi} \right)^{0.15} \), and vice versa for mode \( q_4 \). Regarding that \( \Delta_{\varphi_0} \in [0.85, 1.15] \), we have \( u \in [0.9793, 1.0247] \). For the rest of modes other than \( q_1 \) and \( q_4 \), all continuous inputs, \( u \) and \( \Delta \), are equal to one, i.e. \( u_{\eta_1} = u_{\eta_2} = 1 \) and \( \Delta_{\text{ads}} = \Delta_{\text{prg}} = 1 \) \( \forall q \in \{q_2, q_3, q_5, q_6\} \).

The physical states of the model (7)–(9) at the beginning of each mode are equal to those at the end of the previous mode, whereas the timer \( \tau_c \) resets to \( \tau_c = 0 \) by any mode transition.

3. PSA process as a hybrid system

The two-bed, six-step PSA process described in the previous section is now modeled as a Hybrid Automaton, which is illustrated in Fig. 4. The continuous evolution of the hybrid model in each discrete mode of the process is described by the LROM. The hybrid model of the process is represented as a tuple \( \mathcal{H} = \{X, Q, D, \Sigma, \mu, f, \text{Init, Dom, E, G, } R\} \), where

- \( X = \mathbb{R}^n_{\geq 0} \) is the set of continuous states that are all non-negative. For the two-bed case study there are two physical continuous states corresponding to two adsorption beds along with a state for the timer, then \( n = 3 \);
- \( Q = \{q_i, i \in J\}, J = \{1, 2, \ldots, N_{\text{mode}}\} \) is the set of discrete states. For the six-step process, with respect to Fig. 4, we have \( q_1 = \text{ADS}, q_2 = \text{DPE}, q_3 = \text{BDN}, q_4 = \text{REP}, q_5 = \text{PEQ}, q_6 = \text{REP}, q_7 = \text{BDN} \), where the first and second components of \( q_i \) denote the active cycle-step of BED1 and BED2, respectively;
- \( D \) is the set of continuous disturbances, which includes the variations of the flow rate \( Q_0 \) and the composition \( \varphi \) of Feed stream with respect to their nominal values. As mentioned before, \( \Delta_0 \in [0.9689, 1.0248] \) and \( \Delta_\eta \in [0.9925, 1.0070] \), and then \( D = [0.9689, 1.0248] \times [0.9925, 1.0070] \);
- \( \Sigma = \{\text{trans}, \epsilon\} \) is the set of discrete control events \( \sigma_\epsilon \), where \( \text{trans} \) makes the system transition to the next mode and \( \epsilon \) denotes silence of the controller while no transition is required;
3.1. Performance Tests

- The program was verified on a Sun Enterprise 4100 running Solaris 2.7.
- The computers were connected by a 100 Mbit/s Ethernet switch.
- The experiments were conducted over two different days.

3.2. Results

The results showed that the program was able to complete the tasks within the expected time frames.

Table 1: This table shows the performance of the program with different input conditions.

<table>
<thead>
<tr>
<th>Input Condition</th>
<th>Time (sec)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>12.3</td>
</tr>
<tr>
<td>B</td>
<td>14.7</td>
</tr>
<tr>
<td>C</td>
<td>16.5</td>
</tr>
<tr>
<td>D</td>
<td>18.2</td>
</tr>
</tbody>
</table>

4. Safety Analysis

4.1. Formulation of the safety problem

The safety problem is to identify the conditions under which the system can operate without causing harm.

4.2. Hybrid reachability analysis

Hybrid reachability analysis is a method to determine the possible states that a hybrid system can reach.

- The analysis involves modeling the system as a hybrid automaton.
- This automaton includes both discrete and continuous states.
- The reachability analysis is performed on the hybrid automaton to determine all reachable states.

4.3. Conclusions

The hybrid reachability analysis showed that the system can safely operate within the defined boundaries.

Table 2: This table shows the performance of the program with different input conditions.

<table>
<thead>
<tr>
<th>Input Condition</th>
<th>Time (sec)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>12.3</td>
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<tr>
<td>B</td>
<td>14.7</td>
</tr>
<tr>
<td>C</td>
<td>16.5</td>
</tr>
<tr>
<td>D</td>
<td>18.2</td>
</tr>
</tbody>
</table>

5. Conclusion

The analysis showed that the system is safe and can be operated under the specified conditions.

Acknowledgments

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References


tuous states evolve based on the inputs selected by the players. By implementing such a game for finite automata and continuous dynamical systems, the optimal control laws for the players and the HJI PDE whose viscosity solution describes the boundaries of unsafe sets, are obtained. This procedure has found practical applications in various areas, e.g. Balluchi et al. (2000) and Bayen et al. (2007).

In the two-bed, six-step case study PSA process, we have discrete-event control \( \sigma_c \in \Sigma_c \), continuous control input \( u \in \mathcal{U} \), and continuous disturbance \( \Delta \in \mathcal{D} \). The general procedure introduced by Tomlin et al. (1998) is modified for applying it to our case study hybrid system \( \mathcal{H} \). Consider \( K, \tilde{\mathcal{K}} \), and \( \mathcal{E} \) the subsets of \( X \times Q \), and \( K \) the complement set of \( K \). The controllable predecessor operator \( \text{Pre}_{c}(\cdot) \) applied on \( K \) returns all states of \( K \) for which the controllable actions \( \sigma_c \) can force the states to remain in \( K \) for at least one step in the discrete evolution. The uncontrollable predecessor operator \( \text{Pre}_{d}(\cdot) \) on \( K \) calculates all uncontrollable predecessors of \( K \), i.e. all states in \( \tilde{K} \) along with all states in \( K \) from which the control actions \( \sigma_c \) are not able to maintain the states inside \( K \). The reach-avoid operator \( R.A(\cdot, \cdot) \) applied on the reach set \( \mathcal{G} \) and the avoid set \( \mathcal{E} \), determines the set of all states from which for all \( u \in \mathcal{U} \) there exists a \( \Delta \in \mathcal{D} \) that can drive the state trajectory \( (\mathbf{x}(t), q(t)) \) of execution \( \mathcal{X} \) into the unsafe set \( \mathcal{G} \) without entering the safe set \( \mathcal{E} \). Then the three key operators are

\[
\begin{align*}
\text{Pre}_{c}(K) &= \{ (x, q) \in K : \exists \sigma_c \in \Sigma_c, (x, q', x) \in K \}, \\
\text{Pre}_{d}(K) &= \{ (x, q) \in K : \forall \sigma_c \in \Sigma_c, (x, q', x) \in \tilde{K} \cup K \}, \\
R.A(\mathcal{G}, \mathcal{E}) &= \{ (x, q) \in X \times Q : \forall u \in \mathcal{U}, \Delta \in \mathcal{D} \tilde{\mathcal{E}} \} \\
\begin{cases} 
(x(t), q) \in \mathcal{G} \ 	ext{and} \\
vt \in \{0, 1\} | (x(t), q) \notin \mathcal{E} 
\end{cases}
\end{align*}
\]

and the maximal safe set is calculated by the following recursion (Tomlin et al., 1998):

- **Initialize** \( \Psi^0 = \Omega \); \( \Psi^k = \emptyset \); \( k = 0 \);
- while \( \Psi^k \neq \Psi^{k+1} \)
  - \( \Psi^{k+1} = \Psi^k \cup \text{Pre}_{c}(\Psi^k) \cup \text{Pre}_{d}(\Psi^k) \);
  - \( k = k + 1 \);
- end while \( \Psi^* = \Psi^k \);

The recursion starts with \( \Psi^0 = \Omega \). In each iteration, hybrid reachability of all the unsafe sets is determined by the reach-avoid operator \( R.A(\text{Pre}_{c}(\Psi^k), \text{Pre}_{d}(\Psi^k)) \) and is excluded from the safe area \( \Psi^k \). Finally, at the fixed point of the recursion, a set \( \Psi^* \) will be obtained that is guaranteed to be safe.

To calculate \( \text{Pre}_{c}(\cdot) \) and \( \text{Pre}_{d}(\cdot) \), inversion of the reset function \( \mathcal{R} \) with respect to the quantifiers \( \exists \) and \( \forall \) is required. The computation of the reach-avoid set \( R.A(\cdot, \cdot) \) is the most challenging part of the reported procedure. This computation is conducted by representing the continuous backward reachability problem as a HJI PDE resulted based on a two-player differential game between the continuous controllers \( u \) and the continuous disturbances \( \Delta \):

\[
\frac{\partial \phi(x, \Delta, u)}{\partial t} = \min(0, H^*(x, \lambda))
\]

where \( \phi(x, \Delta, u) \) is the implicit function representing the boundaries of the backward reachable set, \( \dot{\lambda} = \frac{\partial \phi(x, \Delta, u)}{\partial x} \) denotes the spatial derivative of \( \phi \), and \( H^*(x, \lambda, \Delta, u) = \dot{\lambda}^T x \) is the Hamiltonian function, and

\[
H^*(x, \lambda, \Delta, u) = \max_{u \in \mathcal{U}} \min_{\Delta \in \mathcal{D}} H(x, \lambda, \Delta, u)
\]

is the optimal Hamiltonian. The optimal inputs of the two players \( u \) and \( \Delta \) can be calculated respectively by

\[
\begin{align*}
U^* &= \arg \max_{u \in \mathcal{U}} \min_{\Delta \in \mathcal{D}} H(x, \lambda, \Delta, u), \\
\Delta^* &= \arg \min_{\Delta \in \mathcal{D}} H(x, \lambda, \Delta, u^*).
\end{align*}
\]

With regard to the two-player game between the controller (Player I) and the disturbance (Player II), the notation \( \max_{u} \min_{\Delta} \) in Eq. (13) means that Player I plays first, hence, Player II has the advantage since it has prior knowledge of the action of Player I when making its own choice.

### 4.3. Numerical implementation of the hybrid reachability analysis

The viscosity solution of the HJI PDE provides an implicit surface representation of the continuous backward reachable set. Subsequently the backward reachable sets can be computed by the use of level set method that is well studied for approximation of the viscosity solution for time-dependent HJI PDEs (Osher and Fedkiw, 2002). The numerical solution of the HJI PDE, is implemented by using a mildly modified version of an open-source code provided by Mitchell (2004) and Mitchell et al. (2005). The solution is based on the method of lines (MOL) with spatial discretization by weighted essentially non-oscillatory (WENO) scheme (Osher and Fedkiw, 2002). A \( n \)-dimensional uniform Cartesian mesh with fixed grid points is considered, where \( n \) is the dimension of \( x \). First, the PDE is converted to a set of ODEs that are describing the HJI PDE at the defined grid points, and then the numerical integration in time for the obtained ODEs is implemented by Runge–Kutta (RK) method. The optimal Hamiltonian \( H^*(x, \lambda) \) is approximated by the numerical Hamiltonian \( \hat{H}(x, \lambda^+, \lambda^-) \) at each grid point by using the well-known Lax–Friedrichs scheme (Osher and Shu, 1991):

\[
H^*(x, \lambda) = \hat{H}(x, \lambda^+, \lambda^-) = H^*(x, \frac{\lambda^+ + \lambda^-}{2}) - \alpha^T \left[ \frac{\lambda^+ - \lambda^-}{2} \right]
\]

where \( \alpha_i = \max_{\lambda \in \Lambda} \left| \frac{\partial H^*(x, \lambda)}{\partial \lambda_i} \right| \) are the dissipation coefficients with \( \Lambda = \{ \lambda \in \mathbb{R}^n : \lambda^+ \leq \lambda \leq \lambda^- \} \).

For the maximal safe set computation, the calculation of \( \text{Pre}_{c}(\cdot) \) and \( \text{Pre}_{d}(\cdot) \) is performed manually for each iteration. Inversion of the reset function \( \mathcal{R} \) along with knowledge of the mode sequence of the process is required for these calculations. Due to the cyclic operation of the process, the mode sequence is known and fixed as it can be seen in Fig. 4, and then the previous mode of each mode is known. Moreover, the reset function just resets the timer \( \tau_c \) to zero, and does not affect the physical states. Consequently the reach-avoid set \( R.A(\text{Pre}_{c}(\Psi^k), \text{Pre}_{d}(\Psi^k)) \) can be computed by backward reachability analysis.

### 5. Results and discussion

The numerical Hamiltonian is constructed for the different modes of the hybrid system. For instance consider mode \( q_1 \). The Hamiltonian associated to the process dynamics (7)–(9) in this mode is

\[
\begin{align*}
H_{q_1}(x, \lambda, \Delta, u) &= \lambda^T f(x, \Delta, u) = \lambda_1 x_1 + \lambda_2 x_2 + \lambda_3 \tau_c \\
&= \lambda_1 K_{DF} \left( \frac{\dot{q}_2 y_{2.1}(x)}{\lambda_2 q_{12} \lambda_3} - x_1 \right) + \lambda_2 K_{DF} \left( \frac{\dot{q}_2 y_{2.2}(x)}{\lambda_2 q_{12} \lambda_3} - x_2 \right) + \lambda_3.
\end{align*}
\]
To obtain the optimal Hamiltonian $H_{q_1}^*(x, \lambda) = H_{q_1}(x, \lambda, \Delta^*, u^*)$, the optimal inputs $u^*$, $\Delta_{q_1}^*$, and $\Delta_{y}^*$ have to be calculated. During mode $q_1$, BED1 is at the higher pressure and the loading value is increasing while BED2 is being purged at the lower pressure, then $\dot{x}_1 \geq 0$ and $x_2 \leq 0$. With respect to that $x_2 \leq 0$, it is obvious from the equation of $H_{q_1}$ that

$$u^* = \begin{cases} \dot{u} & \text{if } \lambda_2 \geq 0 \\ u & \text{if } \lambda_2 < 0. \end{cases}$$

On the other hand, since $x_1 \geq 0$, by analytical analysis of $H_{q_1}$, in the operating domain of the state variables, the optimal disturbances are

$$\Delta_{y}^* = \begin{cases} \dot{\Delta}_y & \text{if } \lambda_1 < 0 \\ \Delta_y & \text{if } \lambda_1 \geq 0, \end{cases}$$

$$\Delta_{y}^* = \begin{cases} \dot{\Delta}_y & \text{if } \lambda_1 < 0 \\ \Delta_y & \text{if } \lambda_1 \geq 0. \end{cases}$$

Then the optimal Hamiltonian is $H_{q_1}^*(x, \lambda) = H_{q_1}(x, \lambda, \Delta^*, u^*)$ and the dissipation coefficients are

$$\alpha_{1,q_1} = KLDF \left( \frac{a_{y_q_1}(x_1)P_{q_1} \Delta_{Q_1} \Delta_{y} - x_1}{1 + b_{y_q_1}(x_1)P_{q_1} \Delta_{Q_1} \Delta_{y}} \right),$$

$$\alpha_{2,q_1} = -KLDF \left( \frac{a_{y_{q_2}}(x_2)P_{q_2} \Delta_{Q_2} \Delta_{y} - x_2}{\Delta_{Q_1} + b_{y_{q_2}}(x_2)P_{q_2} \Delta_{y}} \right),$$

$$\alpha_{3,q_1} = 1.$$

The numerical equations for the remaining modes can be obtained similarly to those of mode $q_1$. It should be noted that for the modes with timed transitions, i.e. $q_2$, $q_3$, $q_5$, and $q_6$, there are no control inputs and disturbances, and the pressures are time-varying. For the backward reachability analysis, the time-varying pressures $P(t)$ should be implemented backwards in time. In this regard, the pressure ODE in Eq. (3) is solved analytically and is used in numerical Hamiltonian at each time with respect to the back-
ward time $\bar{t} = t - \tau_c$, where $t = 12.1$ s is the duration of the timed modes.

The purity set-point is selected to be $P_{\text{Purp}} = 0.99$ which leads us to the state threshold $Q_{10} = 0.75$ mol/kg. Feed flow rate ($Q_i$) and feed mole fraction of CH$_4$ ($y_i$) are the continuous disturbances and the PFR ($r_{pf}$) is the continuous control input. The inputs $Q_i$, $y_i$, and $r_{pf}$ can range within the intervals of $\pm 25\%$, $\pm 8\%$, and $\pm 15\%$ of their nominal values, respectively. The nominal value of switching times for modes $q_1$ and $q_4$, corresponding to the set-point $P_{\text{Purp}} = 0.99$ at the normal CSS condition, is $\tau_{e0} = 49.6$ s. The switching times of $q_1$ and $q_4$ are considered to be changing in a $\pm 40\%$ interval around $\tau_{e0}$, i.e. $\tau_{e1}^1 = \tau_{e2}^1 = 29.76$ s and $\tau_{e1}^4 = \tau_{e2}^4 = 69.44$ s.

The maximal safe set is computed for the described PSA process. It should be noted that all state variables of the process are non-negative, but some negative states are included in the numerical analysis to ensure that the state constraints at $x = 0$ are satisfied. Furthermore, due to the phase shifted operation of the two adsorption beds in the case study PSA process, the associated cycle-step of the two beds is the same but mirror of each other (see Figs. 2 and 4). Hence, for continuous reachability analysis in each iteration, we can perform the backward computation results only for modes $q_1$, $q_6$, and $q_5$ and the results for $q_4$, $q_3$, and $q_2$, respectively are the same but are mirrored with respect to the dimensions $x_1 = \bar{Q}_2^1$ and $x_2 = \bar{Q}_2^2$. The grids number for the first and second dimensions ($\bar{Q}_2^1$ and $\bar{Q}_2^2$) is 100 grids and it is 100 and 25 grids for the third dimension ($\tau_e$) in the controlled ($q_1$ and $q_4$) and timed ($q_2$, $q_1$, $q_5$, and $q_6$) modes, respectively. Accordingly we have 1,000,000 and 250,000 grid points for the controlled and timed modes, respectively, to be considered in each mode and each iteration of the maximal safe set computation. The numerical solution is implemented in MATLAB® having Mitchell (2004)'s toolbox installed. The corresponding codes are available as supplemental material attached to this paper. The computations in each iteration takes about 56 min on an Intel Core i7-4500U CPU @ 1.80 GHz with 4 MB cache and 6 GB RAM. A fixed point is reached after six iterations. The computed maximal safe set is illustrated in Figs. 5 and 6. To increase the readability of Fig. 5 for modes $q_2$, $q_3$, $q_5$, and $q_6$, the zero boundaries at $\tau_e = 0$ and $Q_{10}^2 = 0$ are not shown.

The process trajectories are guaranteed to be safe with respect to $\Omega$ if they are inside the shown envelopes in Fig. 5, which demonstrate the boundaries of the maximal safe set. Evolution of the continuous states starts at $\tau_e = 0$ in all modes. In modes $q_2$, $q_3$, $q_5$, and $q_6$, the evolution ends up at the top of the envelop at $\tau_e = 12.1$ s, where a timed mode transition occurs. The process trajectories inside the safe sets are not necessarily similar to those on the safe sets' boundaries. In the timed modes, the loading value ($Q_{10}^2$) in the adsorption bed which is undergoing DPE or BDN, reduces, while $Q_{10}^2$ in the other bed, which is in PEQ or REP (respectively), increases. However, it is well-known that there are lower and upper limits on $Q_{10}^2$'s in the mentioned cycle-steps, which are revealed in the resulted maximal safe sets. All state trajectories always remain inside the safe sets. In the controlled modes, $q_1$ and $q_4$, the continuous states evolve according to the process dynamics and the continuous control actions and disturbances, until the control event $\sigma_e$ acts and switches the process mode. It can be seen in the safe set of mode $q_1$ that $Q_{10}^2$ of BED1, which is in ADS step, is increasing over time, while $Q_{10}^2$ of BED2, which is undergoing PRG, is decreasing.

Fig. 6 is a two-dimensional projection of the maximal safe set that shows the initial and target safe sets in each mode of the process in the physical two-dimensional space of $\bar{Q}_2^1$-$\bar{Q}_2^2$. The process trajectory in each mode starts within the initial set and ends up within the target set. In the two-dimensional space in Fig. 6, the shape of the target set in modes $q_1$ and $q_4$ is a one-corner filleted rectangle (semi-rectangle). It is obvious in Figs. 5 and 6 that after a transition from $q_1$ to $q_4$, when the timer $\tau_e$ resets to $\tau_e = 0$, the initial physical states in $q_4$, which are equal to those at the end of $q_1$, remain within the safe set. Based on the obtained maximal safe set, the hybrid controller for modes $q_1$ and $q_4$ can be designed, as well, the safety of the timed transitions in modes $q_2$, $q_3$, $q_5$, and $q_6$ is verified.

In order to show the effect of the continuous inputs of the process on the maximal safe set, the variation intervals of the control input and the disturbances is changed and the maximal safe set is recomputed. The obtained results for mode $q_1$ are illustrated in Fig. 7. It is obvious that increasing the maximum variation interval of the disturbances makes them stronger which shrinks the maximal safe set. On the opposite side, stronger control input makes the maximal safe set extended. Indeed, as it is expected, stronger
controllers and weaker disturbances increase the size of maximal safe set and allow more flexibility in satisfying the lower priority specifications like product recovery.

From the controller design point of view, for instance consider the maximal safe set in mode $q_1$, which is shown in Fig. 8, along with the enabling and forcing boundaries of the control action $\sigma_k$, which are shown by the solid semi-hyperrectangle, named $\mathcal{S}$. In mode $q_1$, BED1 and BED2 are undergoing ADS and PRG steps, respectively. Starting from the safe set at $t_0 = 0$ in mode $q_1$, the process trajectory may enter into $\mathcal{S}$ only from three faces: $f_1$, $f_2$, and $f_3$; although by continuing the evolution, the process trajectory can touch one of the other three faces of $\mathcal{S}$, i.e. $f_4$, $f_5$, and $f_6$. This is due to the fact that in this mode, $Q_1^1$ of BED1 and $Q_2^1$ of BED2 are monotonically increasing and decreasing over time, respectively. The faces $f_1$, $f_2$, and $f_3$ are enabling boundaries and the remaining faces are forcing boundaries. Before the process trajectory reaches the enabling boundaries, the controller is disabled. In this condition, BED1 in ADS step is in safety since the product purity is obviously more than the purity threshold, but BED2, which is undergoing PRG step, needs more time to be regenerated properly. Mode transition in this condition is not safe and will lead to unsafety in the next mode, hence the controller is disabled. At the enabling boundaries, the controller is enabled to change the active mode at any time. Here BED1 and BED2 are both in safety since the purity threshold is satisfied and BED2 is sufficiently regenerated. The controller remains enabled until the process trajectory reaches the forcing boundaries, i.e. $f_4$, $f_5$, and $f_6$, where the controller is forced to change the active mode, otherwise the trajectory goes unsafe immediately. Violating the forcing boundaries leads to unsafe product purity of BED1, although BED2 is perfectly purged and is completely safe.

Inside the boundaries of $\mathcal{S}$, where the safety properties are satisfied, the controller is enabled to act, otherwise, the controller is not allowed to change the mode of the process. As it is mentioned before, in order to select the most appropriate control actions inside the safe region $\mathcal{S}$, the efficiency specifications such as product recovery and process productivity can be taken into account.

6. Conclusions

After introducing mechanistic PDAE model as a full-order model for PSA processes, a LROM was developed based on the full-order model. Then the process was formalized in the framework of hybrid systems and the purity control problem for PSA processes was represented as a safety problem. By means of hybrid reachability analysis the maximal safe set of the process was computed. To the best of our knowledge, this work on reachability analysis of hybrid and distributed parameter chemical processes is the first of its kind. Synthesis of a hybrid controller for PSA processes based on the computed maximal safe set will be the focus of the future work by the authors.

Further studies on challenges and limitations of numerical and practical implementation of the reachability analysis on PSA processes might be of interest. The development of minimal and computationally efficient models that can properly describe the relationship between the measured outputs and the state variables at arbitrary locations of the beds, can be very helpful for estimation of the state variables and for synthesis of the controllers.

Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at https://doi.org/10.1016/j.compecchem.2017.11.007.

References


