ABSTRACT: Tank changeover is a routine process in industry for placing fuel tanks into or out of service. The operation must use inert gas to avoid the flammability zone. However, inert gas consumption should be minimized for economic reasons. This requires dynamic modeling and optimization of the process, as addressed in the present work. A new dynamic optimization problem for minimizing the inert gas consumption, while ensuring fire safety is proposed. As part of the problem constraints, the flammability zone is characterized by disjunctive constraints, which are then converted to a new simple, nonsmooth formula, removing the need for data regression. This together with the multi-mode flow equations in the model leads to a nonsmooth dynamic optimization problem. To enable reliable solution by gradient-based solvers, the problem is reformulated to a smooth one using sigmoid functions. Case studies of methane tank purging and filling operations demonstrate that the proposed approach is able to minimize the inert consumption by providing optimal trajectories of the tank inlet and outlet flow rates, while ensuring the operation remains outside the flammability zone. It is shown that the proposed dynamic optimization can yield significant economic benefits as it reduces the nitrogen consumption by about two-third in one of the examples solved.

1. INTRODUCTION

Safety is a major concern in the operation of chemical plants, where various forms of hazards including fire, explosion, and toxic release are present. It is understood that safety incidents are more likely to happen during process transient conditions such as startup, shutdown, and changeovers, where the process may be subject to uncontrolled changes and unforeseen situations such as equipment malfunctions. Process transitions should be carried out according to prescribed procedures for how the plant variables such as valve openings or flow rates should change with time so that hazardous situations are avoided. Designing an operational procedure for safe transitions requires experience, understanding of the underlying phenomena, and engineering calculations.

An important hazardous situation during process transitions is the buildup of flammable mixtures inside process equipment. This could happen during a vessel changeover, that is, when a vessel designed for storing flammable gases is being taken out of service or brought back to service. The former involves replacing the flammable gas with air, while the latter involves the reverse operation. In both cases, the operation must be performed safely so that the flammable gas/air mixture does not end up with fire or explosion; a situation that could lead to serious property or human losses, as reported in a number of case histories. A safe changeover involves diluting the flammable content by an inert gas such as nitrogen or carbon dioxide such that the mixture composition is kept away from the so-called flammability zone.

The design of safe operating procedures is typically handled by expert plant engineers that mostly rely on their experience and established techniques. For changeover, common techniques include vacuum purging, pressure purging, and sweep-through purging. In general, however, these techniques are not optimal economically and can lead to overuse of the inert component. While safety is of the utmost importance in a changeover operation, it is desirable to reduce the cost by using less amounts of inert. Therefore, a great potential exists in addressing safe changeover operations using optimization techniques.

The conservative nature of safety problems makes it challenging to devise an operation path that minimizes the inert consumption while ensuring safety of the process. This work aims to address this challenge through the systematic approach of mathematical programming. In particular, the
objective is to find the flow trajectories of the incoming and outgoing gases to/from the vessel that minimize the inert consumption and avoid running into the flammability zone. The focus is on the sweep-through procedure as it is the most flexible in terms of flow adjustments and that the other two procedures can be seen as its special types. To author’s best knowledge, only limited work has been carried out on the application of optimization to this problem so far.

There are a number of mathematical difficulties associated with optimizing a changeover operation. First, the operation is inherently dynamic. Therefore, the optimization involves dealing with a dynamic model and finding the best trajectories of the decision variables, which is essentially an infinite dimensional search. Second, the inlet and outlet flow rates can exhibit multiple operating modes depending on the relative upstream and downstream pressures. For example, the flow could switch from normal to choked or even zero flow during the operation. These switches give rise to discrete events in the underlying dynamic model, leading to a hybrid discrete-continuous dynamic system. In modeling of chemical engineering-processes, hybrid dynamic models arise frequently as a result of discrete events in the internal physico-chemical processes such as switches in the phase regime (e.g., vapor to vapor−liquid) and flow direction (i.e., flow reversal) or in external actions such as triggering of a safety relief valve. The simulation and optimization of hybrid dynamic systems have been studied extensively (see e.g., Stechlinski et al., Galán et al., Barton et al., Barton and Lee, and Khan et al.). Arguably, the theory for the simulation of hybrid dynamic systems is at a state of maturity, and solid software packages exist for this purpose (see e.g., DAEPACK/JACOBIAN and gPROMS). However, optimization of such systems remains a challenging task both theoretically and practically. The main reason is that the functions involved in the dynamic model often lose their differentiability due to the discrete events. Consequently, the entire dynamic model is not guaranteed to be differentiable with respect to its inputs unless strict conditions are met. Therefore, gradient-based optimization algorithms may not be used reliably for optimizing hybrid dynamic systems. Specifically, these algorithms may converge to a sub-optimal solution or not converge at all.

The non-differentiability of the changeover process model comes from explicit inclusion of normal, choked, and zero flow in the model, as recognized in a study by Barton et al., where a formulation for optimizing the process was also proposed and solved. However, the process considered in the study by Barton et al. has several differences with that considered here. First, in the study by Barton et al., a tank full of fuel is to be filled with oxygen, rather than air or inert as common in vessel purging operations. Second, the control valves in the study by Barton et al. are assumed to take on/off positions only. Third, from an optimization standpoint, the objective function in the study by Barton et al. is to minimize the duration of the operation, rather than inert consumption. Moreover, the authors resort to a stochastic optimization method due to the problem’s non-differentiability. Unlike gradient-based methods, however, stochastic methods are computationally intensive and cannot provide a mathematical guarantee of optimally unless run for an indefinitely long time. A similar changeover problem has been addressed in Asprey et al., where propylene and steam are considered as the fuel and inert, respectively. Instead of on/off valves, the inlet valves are allowed to take multiple prescribed, discrete positions. However, the system has been simplified by assuming that the vessel pressure, and in turn, holdup are constant. Also, the choked flow is not accounted for in the model. The optimization is then broken into two sequential layers, where the time minimization problem is carried out in the first layer using stochastic search, and the safety constraint is handled in the second layer. The same propylene/air/steam system with a constant pressure and holdup assumption has also been optimized in Batres. The optimization problem is solved again by stochastic search (i.e., a modified genetic algorithm). More recently, a time-optimal changeover problem for the methane/nitrogen/oxygen mixture, as mentioned in the study by Barton et al., has been addressed in a study by Fakhroeslam et al. via a symbolic control approach. The system still uses on/off valves and assumes constant vessel pressure and holdup. Apart from these simplifying assumptions, the symbolic model approach is meant for online control applications, rather than offline prescription of optimal trajectories as pursued in this work. Moreover, the construction of the symbolic model, which is carried out offline, is inherently a complex task and involves approximation of the original dynamic model. Therefore, the symbolic approach would not be justified for the present work, where optimal process trajectories can be best achieved using direct optimization of an accurate dynamic process model.

It is seen that in all the abovementioned studies, the objective is to complete the changeover in the shortest time possible. Nonetheless, tank changeover is typically not an emergency operation, where a quick response may be important. Even if an emergency changeover is required, there is no time for pre-planning using offline optimization due to the spontaneous nature of emergency situations. Therefore, to obtain minimal time using offline optimization in an emergency response would not be relevant in the first place. In such situations, the most practical approach is perhaps to use the highest amount of inert. Considering the fact that tank changeover is typically a routine operation, where planning is possible, and that gas systems are relatively quick already, it can be argued that what matters more than time is the cost of the operation as implied by the amount of the inert consumed. Also, most of the previous work make some simplifying assumptions (such as on/off valves and constant pressure) that would make the problem less realistic.

In response to the abovementioned gaps, this work presents a new dynamic optimization formulation for inert minimization during changeover operations. Similar to Barton et al., all flow conditions, namely normal, choked, and zero flow in the case of back pressure, are taken into account explicitly in the model. Moreover, the valves are not constrained to take only a limited number of positions and can take any value between 0 and 100%. Both filling and purging operations are accommodated in the proposed formulation. Another contribution of this work is a new method for characterization of the flammability zone that is simple and removes the need for data regression or conjunctive relations. In particular, the flammability zone is represented by the so-called mid function that recently has been used frequently for nonsmooth, yet continuous, reformulation of conjunctive relations such as equilibrium phases. An important advantage of the new characterization method is that it requires minimal flammability information. Therefore, it is still applicable when lack of sufficient flammability data makes it impractical to characterize the flammability zone using regression methods or when it is impossible or hard to find an appropriate fitting function to use in the regression. The nonsmooth flammability zone representation together with the discrete flow switches result in a generally non-differentiable dynamic optimization
problem. Unlike previous work, however, the problem is solved using gradient-based optimization methods that are able to prove local optimality. This is accomplished by reformulation of the originally nonsmooth problem into a smooth one using sigmoid functions, a simple alternative to complicated reformulations (see Subsection 3.3). The novelties of this work can be summarized as follows: (i) proposing a more realistic formulation for the optimal changeover operation, (ii) proposing a new approach to over-approximation of the flammability zone that works with minimal flammability data, and (iii) amending the resulting (generally) non-differentiable problem to gradient-based optimization algorithms using a smooth reformulation.

The remainder of the paper is organized as follows. In Section 2, the changeover problem and its hybrid dynamic model are presented formally. The dynamic optimization problem is formulated, and its features are discussed in Section 3, where more technical details for the interested reader on challenges of solving the resulting non-differentiable optimization problem are also presented in Subsection 3.3. This paves the way for presenting the proposed smooth reformulation in Section 4. The effectiveness of the proposed dynamic optimization approach and its economic merits are demonstrated through case studies in Section 5. Finally, conclusions are provided in Section 6.

2. SAFE TANK CHANGEOVER

In a changeover operation, fuel tanks that are initially full of air/inert are put in service by replacing the content with fuel (e.g., during plant startup). Similarly, the tanks are placed out of service by replacing the fuel content with air/inert (e.g., during shutdown). In both changeover operations, it is important to avoid forming a flammable air/fuel mixture, else an explosion could result. The flammable mixture is characterized by the flammability zone, as shown schematically in the ternary plot of fuel, oxygen, and nitrogen in Figure 1. Any changeover operation must avoid the flammability zone. Also shown in Figure 1 is the path of moving from a tank full of fuel (point A) to one full of air (point B) or vice versa without using additional inert. This is called the air line. Clearly, this path crosses the flammability zone, posing the risk of fire or explosion. Therefore, an inert gas (e.g., nitrogen) must be added in order to keep the air/fuel compositions in the tank outside the flammability zone.

The tank changeover system is illustrated in Figure 2. During the changeover operation, all the three inlet and the outlet flow rates are allowed to be adjusted in the interest of avoiding the flammability zone. From an economic perspective, it is also desirable to minimize the inert consumption. This motivates mathematical optimization for finding the best flow rate trajectories during the operation. A key requirement for the optimization is availability of a dynamic model for the changeover process, which is discussed in the following subsection.

2.1. Dynamic Modeling. For simplicity, an isothermal process and ideal gas conditions are assumed. These assumptions can be relaxed by making appropriate changes to the thermodynamics without impacting the arguments presented in this paper. This is because the main objective here is the formulation and reliable solution of the optimal changeover problem, which can be applied to models with different levels of physical rigorosity. For purpose of the ensuing developments, the dynamic model of the changeover operation for methane is adapted from studies by Barton et al. and Yunt. The main change made in this work is that instead of a pure oxygen supply as mentioned in studies by Barton et al. and Yunt, an air supply is considered here (see Figure 2). This makes the setup more industrially relevant and consistent with the practical objectives of purging or filling a tank with fuel. The resulting dynamic model is in the form of differential algebraic equations (DAEs) as follows.

\[
\hat{n}_i(t) = \sum_{j=1}^{3} F_j(t) y_{i,j} - F_i(t) y_{i,A}(t), \quad \forall \ i = 1, 2, 3 \quad (1)
\]

\[
\forall \ t \in (t_0, t_f]
\]

\[
y_{i,A}(t) = \frac{n_i(t)}{n_T(t)}, \quad \forall \ i = 1, 2, 3, \quad \forall \ t \in [t_0, t_f]
\]

\[
n_T(t) = \sum_{i=1}^{3} n_i(t), \quad \forall \ t \in [t_0, t_f]
\]

\[
P(t) = n_T(t) \frac{RT}{V}, \quad \forall \ t \in [t_0, t_f]
\]

\[
F_i(t) = \begin{cases} 
0 & \text{if } \frac{P(t)}{P_j} \geq 1 \\
\phi_i(t) C_{\phi} \left( \frac{P + P(t)}{2} - \frac{P_j - P(t)}{\sqrt{P_j - P(t) + \eta_j P}} \right) & \text{if } 0.53 \leq \frac{P(t)}{P_j} < 1, \ j = 1, 2, 3 \\
\phi_i(t) C_{\phi} \frac{P}{\sqrt{2}} & \text{if } \frac{P(t)}{P_j} < 0.53 
\end{cases}
\]

\[
(2)
\]
\[
F_j(t) = \begin{cases} 
0 & \text{if } \frac{P_j}{P(t)} \geq 1 \\
\frac{u_j(t)}{C_k}\sqrt{\frac{P(t) + P_j}{2} - \frac{P(t) - P_j}{\sqrt{P(t) + P_j}} - k_bP(t)} & \text{if } 0.53 \leq \frac{P_j}{P(t)} < 1 \\
\frac{u_j(t)}{C_k}\sqrt{\frac{P(t) + P_j}{2} - \frac{P(t) - P_j}{\sqrt{P(t) + P_j}}} & \text{if } \frac{P_j}{P(t)} < 0.53 
\end{cases}
\]

with the initial conditions
\[
n_{\text{CH}_4}(t_0) = n_{\text{CH}_4}^0, \quad n_{\text{O}_2}(t_0) = n_{\text{O}_2}^0, \\
n_{\text{N}_2}(t_0) = n_{\text{N}_2}^0,
\]

where \( R \) [mole m\(^3\) mole\(^{-1}\) K\(^{-1}\)] is the global gas constant; \( n_i \) [mole] and \( y_i \) refer, respectively, to the number of moles and the mole fraction of the component \( i \) \( \in \{ \text{CH}_4, 1, \text{O}_2, 2, \text{N}_2, 3 \} \) in the tank; \( F_j \) [mole s\(^{-1}\)] and \( P_j \) [bar], respectively, denote the flow rate and the known pressure of the \( j \)th inlet stream; \( y_{i,j} \) is the mole fraction of the \( j \)th component in the \( i \)th stream; \( V \) [m\(^3\)]; \( P \) [bar], and \( n_T \) [mole] are the tank volume, total pressure, and total moles inside the tank, respectively; \( u_i \in [0, 1] \) and \( C_{o,j} \) \( j = 1, 2, 3 \) and \( 4 \) [mole s\(^{-1}\) bar\(^{-1}\)] are the valve opening and valve coefficient for the \( j \)th stream, respectively; and \( k_b > 0 \) and \( C_k \) are regularization constants for improving the model's numerical behavior, as discussed in the sequel.

The flow equations 2 and 3 cover three operating modes: zero flow through the valve in the case of a higher downstream pressure (i.e., check valve), normal flow, and choked flow. The inclusion of zero reverse flow and choked flow is very important in modeling the changeover process. Ignoring these phenomena would lead to unrealistic flow patterns, and thus, wrong impression of a safe operation. The \( C_k \) constant ensures continuity of the flow from one mode to another. Also, it should be mentioned that the flow equations have been modified by Barton et al.\(^{19}\) and Yunt\(^{20}\) from their conventional form, which involves the square root of pressure drop across the valve. The modified form has better numerical properties in that the square root argument of the normal flow equation strictly positive.\(^{20}\)

3. OPTIMAL CHANGEOVER FORMULATION

For a purging operation, the objective is to empty the tank from inert gas while minimizing the inert consumption and avoiding the flammability zone during the operation. The valve openings can be manipulated for this purpose. Therefore, the following optimization problem can be formulated.

\[
\min_{u_j(t)} \int_{t_0}^{t_1} F_j(t) dt 
\]

s.t. dynamic model \( (1 - 3) \), \( \forall \ t \in [t_0, t_1] \),
\( y_j(t) \leq y_j^{\text{max}} \) \( (P1.1) \),
\( g(t) \leq 0, \quad \forall \ t \in [t_0, t_1] \) \( (P1.2) \)

\( u_j(t) \in [0,1] \) \( \alpha. e. \ in [t_0, t_1] \)

The objective function in problem P1 gives the total nitrogen used through the inert stream. Constraint P1.1 enforces a fuel content of at most \( y_{i_{\text{max}}} \) in the tank at the end of the operation, and P1.2 is a path constraint that ensures the mixture does not enter the flammability zone at any time during the operation. The vessel pressure cannot exceed the maximum pressure of the inlet streams. This is due to the fact that the inlet streams are pressure-specified, and the incoming flow stops when the pressures equilibrate (see eqs 2 and 3). Therefore, there is no need to add a safety constraint for the vessel pressure if the vessel can already withstand the highest pressure set for the inlets (see the data in Table 2).

Formulation P1 can be used for filling operation with the following changes. First, the fuel content at the end of the operation should be near 100%, that is, constraint P1.1 will be replaced with \( y_{i_{\min}} \). Second, the initial conditions will change to \( n_{\text{CH}_4}(t_0) = 0, n_{\text{O}_2}(t_0) = n_{\text{O}_2}^0, n_{\text{N}_2}(t_0) = n_{\text{N}_2}^0 \), indicating a tank full of oxygen/nitrogen with the air or other compositions. Third, a final-time constraint on the vessel pressure or molar content is enforced to make sure that enough fuel has been stored in the vessel at the end of the operation. Such a constraint could be presented as lower/upper bounds on the vessel molar content or pressure (see Subsection 5.2).

Remark 1. The economic objective here accounts for the inert consumption only. Nevertheless, it may be desired to modify the objective by also accounting for the fuel consumption in the form of the total inert and fuel cost. A difficulty, however, would be access to the relative prices of inert and fuel to be used as weighting factors in the objective function. Such information may not be available with enough certainty to ensure reliable results. It is worth noting that the cost of fuel is not relevant in purging operations because the fuel valve is kept closed (see Section 5), and thus, no fresh fuel is used during the operation. The cost of fuel would be relevant in filling only because the incoming fresh fuel is allowed to exit the tank through the outlet valve during the operation. It should be emphasized that the ensuing developments remain valid regardless of the objective function.

Remark 2. Without loss of generality, the duration of the operation is already decided in Problem P1. It is possible to consider the final time \( t_f \) an additional optimization variable. This would allow more flexibility in choosing the optimal path, hence yielding a better optimal solution potentially. A free final-time optimization can be rewritten as a fixed final-time problem by a simple change of variable, as described in the dynamic optimization literature (e.g., Chachuat\(^{21}\)). It should be emphasized that the proposed approach can easily handle fixed and free final-time formulations.

Arguably, a challenge in problem P1 is how to formulate constraint P1.2, which requires a mathematical characterization of the flammability zone (see Figure 1). It is possible to approximate the boundaries of the flammability zone using polynomial regression.\(^4\) However, besides the difficulty of finding a suitable regression model, the approximation obtained in this way may underestimate the flammability zone. This can lead to a changeover operation that would actually enter the danger zone even if it is deemed to follow a safe path based on the approximated flammability zone. In this work, a simpler approach to characterization of the flammability zone and the...
safe operation path is proposed. This is discussed in the next subsection.

3.1. Characterization of the Safe Operation Zone. A major challenge in characterizing the flammability zone is lack of sufficient experimental data for most flammable gases (see Chapter 6 in the book by Crowl and Louvar\(^{1}\)). This renders regression techniques inapplicable in many cases. Even if sufficient data are available, it may be hard to find an appropriate regression function (e.g., polynomials of some degree or other function forms) that can fit the data satisfactorily. Lack of control on the level of under/over-approximation is another issue with regression as it normally draws a curve through the data points. As discussed in Crowl and Louvar,\(^1\) instead of regression, the flammability zone can be approximated by simpler techniques utilizing only few data points such as the lower-flammability limit and limiting oxygen concentration. These techniques result in intersecting straight lines on the flammability diagram that determine the boundaries of the flammability zone. These lines, as shown schematically by the blue dash-dotted lines in Figure 1, represent an overestimation of the lower and upper boundaries of the flammability zone. This representation lends itself perfectly to disjunctive relations and a nonsmooth reformulation, as presented in the sequel.

As mentioned above, the lower and upper boundaries of the flammability zone are overestimated using the blue dash-dotted lines in Figure 1. The methane mole fractions on these lines are given by

\[
\begin{align*}
\hat{y}_{\text{CH}_4}^U &= a y_{O_2} + b \\
\hat{y}_{\text{CH}_4}^L &= c y_{O_2} + d
\end{align*}
\]  
(4)  
(5)

where the constants \(a, b, c,\) and \(d\) are obtained simply from any two points on the lines. An advantage of characterizing the flammability zone by eqs 4 and 5 over using regression is that the lines can be set such that they guarantee to overestimate the flammability zone. From Figure 1, it is evident that the flammable mixture is outside the approximated flammability zone if

\[
\begin{align*}
\chi_{\text{CH}_4} \geq \hat{y}_{\text{CH}_4}^U, & \quad \text{OR} \\
\chi_{\text{CH}_4} \leq \hat{y}_{\text{CH}_4}^L
\end{align*}
\]  
(6)  
(7)

where OR is the inclusive disjunction as the changeover path is safe if either of the above inequalities holds or they both hold at the same time (note from Figure 1 that \(\hat{y}_{\text{CH}_4}^U\) is not always greater than \(\hat{y}_{\text{CH}_4}^L\)). A difficulty with disjunctive constraints, however, is that they cannot be readily added to the set of constraints in the optimization problem. This is because optimization solvers interpret the set of constraints as conjunctive, that is, they must all hold at the same time for the problem to be feasible. The disjunction inequalities 6 and 7 can be modeled naturally by disjunctive programming techniques.\(^{22}\) Due to its discrete nature,\(^{23}\) however, the solution of a disjunctive program can be computationally expensive, imposing further complexity on the dynamic optimization problem considered in this work. Consequently, the inequalities 6 and 7 must be reformulated to mean conjunction or somehow converted to a single constraint. The solution proposed in this work is presented in the sequel.

3.1.1. Proposed Nonsmooth Characterization of the Safe Operation Zone. Here, a new formulation is proposed for mathematical representation of the safe operation zone while avoiding complications of the disjunctive constraints. Specifically, the two inequalities 6 and 7 are converted into one as

\[
\text{mid}(\chi_{\text{CH}_4} - \hat{y}_{\text{CH}_4}^L, 0, \hat{y}_{\text{CH}_4}^U - \chi_{\text{CH}_4}) \leq 0
\]  
(8)

where mid selects the median of its three arguments. The mid function is a compact form for representing disjunctive constraints and recently has found interesting applications in efficient modeling and optimization of chemical processes involving different operating modes (see e.g., Sahlodin et al., Watson and Barton, Watson et al., Vikse et al., and Cavalcanti and Barton\(^{26}\)). To show how the single inequality 8 correctly represents the exterior of the flammability zone, the ternary plot in Figure 1 is divided into four regions based on the boundaries defined by the lines given in eqs 4 and 5. Then, the sign of the mid function in each region is investigated. As shown in Table 1, the only region where the mid function evaluates to positive (hence violating the inequality 8) is the approximated flammability zone. Therefore, satisfaction of inequality 8 means the operation is safely outside the flammability zone.

Now, the formulation P1 is completed by writing the path constraint P1.2 as

\[
\text{mid}(\chi_{\text{CH}_4}(t) - \hat{y}_{\text{CH}_4}^L(t), 0, \hat{y}_{\text{CH}_4}^U(t) - \chi_{\text{CH}_4}(t)) \leq 0, \\
\forall \ t \in [\tau_0, \tau_1]
\]  
(9)

3.2. Numerical Solution Aspects. The computational aspects of the formulation P1 are discussed in this subsection.

3.2.1. Dynamic Optimization Approach. This work employs deterministic optimization based on gradient-based methods\(^{27}\) for solving P1. A difficulty with solving problem P1 is the infinite-dimensional decision space that results from the optimization over control trajectories. In so-called direct methods for dynamic optimization, this difficulty is overcome by parameterizing the control trajectories over time.\(^{21}\) Piecewise constant parameterization of the control variables into \(N\) equally spaced time intervals is used in this work, as illustrated in Figure 3.

Another complexity is the presence of a nonlinear dynamic model, which cannot be handled explicitly by nonlinear program (NLP) solvers. In the absence of a closed-form solution, the dynamic model in direct methods is tackled by either (i) discretizing the state variables by, for example, collocation methods and introducing additional optimization variables (simultaneous approach) or (ii) resolving the dynamic model using standard numerical integrators (sequential approach).\(^{28}\) In other words, the simultaneous (aka full-discretization)
approach approximates the dynamic model by a set of nonlinear algebraic equations that are added to the set of problem constraints. This removes the need for integration of the dynamic model and enables the robust solution of systems with unstable dynamic systems. On the downside, however, the a priori discretization of the dynamic system in the simultaneous approach results in many new auxiliary variables, leading to a large-scale constrained NLP with potential difficulties finding an appropriate set of initial guesses. On the other hand, the sequential approach employs a numerical integrator to solve the dynamic model accurately without adding any auxiliary variables. This has the advantage of keeping the problem dimension comparatively small and being able to solve large-scale, stiff dynamic models with high accuracy. Therefore, the direct sequential approach is adopted in this work. As illustrated in Figure 4, at each iteration of the sequential approach, the NLP solver calculates a set of trial values for the decision variables. The integrator block then integrates numerically the dynamic model, in which the decision variables serve as constant parameters. The integration results that include values of the state variables are then used to evaluate the objective and constraint functions and check the optimality conditions by the NLP solver.

Figure 3. Discretization of the control variable $u(t)$ into piecewise constant parameters $p_i$, $i = 1, \ldots, N$.

Figure 4. Direct sequential approach to dynamic optimization.

$solver calculates a set of trial values for the decision variables. The integrator block then integrates numerically the dynamic model, in which the decision variables serve as constant parameters. The integration results that include values of the state variables are then used to evaluate the objective and constraint functions and check the optimality conditions by the NLP solver. More information on and comparisons of the simultaneous and sequential approaches can be found in the dynamic optimization literature, for example, studies by Chachuat, Biegler, and Kameswaran and Biegler.

3.2.2. Path Constraint. The safety constraint $g$ must remain satisfied over the entire path of the dynamic operation. Path constraints can be handled numerically by transcription to an equivalent final-time constraint. In particular, an inequality path constraint $g(t) \leq 0$, $\forall t \in [0, t_f]$ is substituted with

$$x_i(t_f) = \int_0^{t_f} [\max(0, g(t))]^2 dt \leq \epsilon$$

where $x_i$ is an auxiliary state variable, and $\epsilon$ is a small positive number used to meet a constraint qualification. The integrand is squared in order to avoid the non-differentiability introduced by the max function.

3.3. Remarks on Problem Differentiability. The eqs 2 and 3 and the path constraint 9 embedded in P1 involve functions defined by conditional statements, representing discrete events that define switches from one mode to another in the dynamic model. This gives rise to a hybrid discrete-continuous dynamic system. As mentioned before, the discrete events generally correspond to kinks in the model, as illustrated for the simple min and max functions in Figure 5, and potentially cause non-differentiability of the overall hybrid system with respect to the decision variables.

Figure 5. Example of min/max functions and their point of non-differentiability.

Conditions for the existence of sensitivities (i.e., derivatives) of hybrid dynamic systems w.r.t. their parameters are investigated in several studies (e.g., Gala et al., Khan et al., Khan and Barton, and Khan et al.). Nonetheless, such conditions are often hard to satisfy or verify a priori and may require reformulation of the model based on further assumptions before the existence of derivatives can be checked or guaranteed (see e.g., Sahlodin and Barton). The lack of sensitivities or uncertainty about their existence creates an obstacle in using gradient-based algorithms for optimization of hybrid dynamic systems. Such algorithms may not converge for a non-differentiable problem, and when they do converge, one cannot be certain about the optimality of the result due to the possibility of wrong search directions. To circumvent the non-differentiability issue, early proposals include reformulation of the mode switches into integer decisions, leading to a mixed-integer dynamic optimization problem (see e.g., Avraam et al., Till et al., and Buss et al.). Although this approach removes the non-differentiability issue, it often leads to many integer variables and a large-scale problem, which is computationally costly to solve. Interested readers are referred to Section 8.4 of Yunt for a computational study of handling the mode switches using the mixed-integer reformulation. An alternative approach is modeling of the discrete events by complementarity constraints, which turn the integer decisions to continuous ones, resulting in an NLP problem. This approach reduces the computational complexity by removing the integer variables. Nonetheless, complementarity constraints by nature cause additional nonlinearity in the problem, increasing the risk of solver failure or solution sub-optimality. Moreover, optimization problems with complementarity constraints are
known to violate constraint qualifications at any feasible point, rendering the well-known KKT conditions as no longer necessary for local optimality. Therefore, optimization of hybrid dynamic systems reformulated by complementarity constraints suffers from yet another complexity as it requires special treatment of these constraints to make them amendable to gradient-based solvers. The treatment strategies include penalizing the objective function with the complementarity constraints or regularizing these constraints by smooth reformulations. These strategies employ a penalization or smoothness parameter for adjusting the degree of approximation. It can be shown that in the limit, the smoothed problem approaches the original hybrid dynamic system.

Despite the abovementioned progress, the reformulation of the switches modeled by complementarity constraints still looks to be a challenging task for the following reasons: (i) the reformulation of the discrete events as complementarity constraints requires special modeling skills on top of the expertise needed for modeling of hybrid dynamic systems; (ii) the complementarity constraints make the problem more constrained, more nonlinear, and generally more non-convex; (iii) the solvability of the dynamic model (especially in the case of DAEs) with complementarity constraints requires certain assumptions to ensure that the model is mathematically well-posed; (iv) the complementarity constraint reformulation alone is not adequate for successful solution of the problem using gradient-based solvers, and regularization of the constraints using, for example, smoothing functions is still necessary. The aforementioned complexities incentivize simpler reformulation strategies for making hybrid dynamic systems amendable to gradient-based solvers. In particular, a direct smoothing approach is presented in this work, where the hybrid dynamics is reformulated by smooth functions without introducing any integer variables or complementarity relations. This seems to be a promising approach, especially for hybrid systems with nonsmooth, but continuous dynamics, as in the changeover process under study. With this approach, the size and the natural form of the dynamic model is retained, making it easier to understand, maintain, and optimize. In the next section, the smooth reformulation of problem P1 is detailed.

4. PROPOSED SMOOTH FORMULATION

There are two sources of potential non-differentiability in P1. One is the eqs 2 and 3 that describe the three modes of no flow, normal flow, and choked flow through the tank’s inlet and outlet streams. The switches between the modes are modeled by conditional statements. However, the flow is inherently a continuous variable, and it is easy to verify that the three flow modes can be represented in a compact form by yet another application of the mid function as

\[
F_j(t) = \text{mid} \left( 0, u_j(t) C_{j+c} \sqrt{ \frac{P_i + P(t)}{2} - \frac{P_i - P(t)}{\sqrt{|P_i - P(t)|} + k_i P_i} + u_j(t) C_{j+c} \frac{P_i}{\sqrt{2}} 0.85 \right)
\]

with \(j = 1, 2, \) and 3. The other source of non-differentiability is the mid function used in the formulation of the path constraint. The mid function can be written as

\[
\text{mid}(a, b, c) = a + b + c - \max(a, b, c) - \min(a, b, c)
\]

\[
= a + b + c - \max(\max(a, b), c) - \min(\min(a, b), c)
\]

The nested min and max functions are evaluated by simply calling the function twice, where the result of the inner function serves as the input argument to the outer function. It is evident from eq 13 that the mid function is a continuous function with points of non-differentiability. Therefore, the dynamic optimization problem P1 is not guaranteed to remain differentiable w.r.t. the optimization variables. Consequently, the derivatives calculated symbolically or estimated via finite differences would not be correct in general. This can cause gradient-based solvers to converge to the wrong solution or not converge at all, adding further complications to an already non-trivial dynamic optimization problem.

To address the above challenge, it is proposed to replace the min and max functions with their smooth approximations. In this way, all the equations involved in the optimization will be differentiable, and the problem can be solved reliably using a gradient-based solver. In particular, the following sigmoid function is employed for this purpose.

\[
S(z) = \frac{1}{1 + e^{-z}}
\]

The min and max functions are then approximated as follows.

\[
\max(a, b) = \frac{a}{1 + e^{-\beta c}} + \frac{b}{1 + e^{-\beta c}}
\]

\[
\min(a, b) = \frac{a}{1 + e^{-\beta c}} + \frac{b}{1 + e^{-\beta c}}
\]

where the accent ~ indicates approximation; \(z := b - a\); and \(\beta\) is a positive parameter used for adjusting the degree of approximation. The approximate min and max functions for different \(\beta\) values are plotted and compared with their exact counterparts in Figure 6. It is seen that around the kink points, the smooth approximations exhibit a small deviation, which can be reduced by increasing \(\beta\). Nonetheless, it should be noted that too large a \(\beta\) would cause numerical difficulties although the problem remains differentiable theoretically.

The approximate mid function is then constructed simply from the approximate min and max functions. As a result, the entire optimization problem is now free of mode switches and can be handled by conventional gradient-based algorithms.

5. RESULTS AND DISCUSSION

In this section, a number of case studies are presented to demonstrate the smooth dynamic optimization for optimal
changeover operations. The proposed optimization problem is solved using the active-set method,\textsuperscript{47} which is a local optimization algorithm, and the underlying DAEs are integrated numerically using the variable-step backward differentiation formula.\textsuperscript{48} Global dynamic optimization algorithms could also be employed; however, it would require the use of techniques for building convex relaxations of the underlying dynamic model, which is beyond the scope of this work (see e.g., Sahlodin and Chachuat\textsuperscript{49,50} and Sahlodin\textsuperscript{51} for details).

The model constants that have been taken from Yunt\textsuperscript{20} are provided in Table 2. The flammability zone for methane (see e.g., Chapter 6 in Crowl and Louvar\textsuperscript{1}) is over-approximated by eqs 4 and 5 with the following constants: $a = 2$, $b = -0.11$, $c = 0$, and $d = 0.03$. These values provide a rather tight approximation of the flammability zone on the bottom and top sides and leave a visible over-approximation toward the left corner of the zone, as seen in for example, Figure 9. If a better safety margin from all sides is desired, the approximation can be inflated by adjusting the above values. The optimization results are presented for two scenarios of placing the vessel out of and into service.

### 5.1. Safe Placing of Vessel Out of Service

Here, the vessel is to be emptied from fuel. The fuel fraction at the end of the purge must not exceed $y_{i_{\text{max}}}$, and the vessel is filled with almost all nitrogen at the end of the operation. The optimal operation path is illustrated in Figure 9, where the methane mole fractions are read from the intersection of the horizontal grid lines with the methane axis, the nitrogen mole fractions are read from the intersection of the grid lines parallel to the oxygen axis with the nitrogen axis, and the oxygen mole fractions are read from the intersection of the grid lines parallel to the methane axis with the oxygen axis. The purging operation starts at $t = 0$ s from the 100% fuel condition, that is, the top vertex in the ternary diagram. The operation path is featured with time markers to show the time trend of the vessel composition. Interestingly, the vessel remains at 100% fuel up to $t = 100$ s. This is explained by the fact that the inlet inert and air valves are both closed up to this time, as shown in Figure 7. It is seen that the operation successfully avoids the over-approximation of the flammability zone (the ternary graphs are plotted using the code provided by Sandrock and Afshari\textsuperscript{52})

As a second experiment, a finer control parameterization with six evenly spaced intervals is adopted. The same smoothness parameter value of $\beta = 2$ is used. The optimal valve openings and

![Figure 6. Min/Max functions and their smooth approximations.](https://example.com-figure6)

![Figure 7. Optimal valve openings and resulting flow rates for placing vessel out of service using the smooth formulation with $N = 3$ and $\beta = 2$.](https://example.com-figure7)

![Figure 8. Optimal trajectories of state variables for placing vessel out of service using the smooth formulation with $N = 3$ and $\beta = 2$.](https://example.com-figure8)

| constant | value | constant | constant | value |
|----------|-------|----------|----------|-------|
| $C_{V,0}$ | 8 mol/s·bar | $R_{0}$ | 12 bar |
| $C_{V,N_2}$ | 8 mol/s·bar | $R_{N_2}$ | 7 bar |
| $C_{V,CH_4}$ | 8 mol/s·bar | $k_{CH_4}$ | 10 bar |
| $C_{V,N_2}$ | 8 mol/s·bar | $P_4$ | 2 bar |
| $T$ | 300 K | $R$ | $8.314 \times 10^5$ bar·m$^3$·mol$^{-1}$·K$^{-1}$ |
| $V$ | 3 m$^3$ | $k_o$ | $10^{-5}$ |

\(^{\text{a}}\text{p.}\)
the corresponding inlet/outlet flow rates are given in Figure 10. The resulting optimal trajectories of the state variables and the optimal operation path are shown in Figures 11 and 12, respectively. The total nitrogen consumption in this case is 674 mol, that is, a 67% decrease compared with the previous case, where a coarser control parameterization was used. A finer control parameterization allows more flexibility in the valve opening and flow rate variations with time, thereby enlarging the feasible search space and potentially improving the optimal solution.

As noted previously, the value of $\beta$ affects the degree of smoothing, and in turn, deviation from the actual switching behavior. Therefore, it is interesting to see how changing $\beta$ would impact the optimal solution. To this end, $\beta$ is reduced to 1, and the optimization with 6 control intervals is repeated. The results are shown in Figures 13–15. The minimum nitrogen usage in this case is obtained as 1256 mol, which is almost twice the case with $\beta = 2$. Both optimization problems with $\beta = 2$ and $\beta = 1$ use 6 control intervals. Therefore, the inferior solution with $\beta$
1 could be attributed to the larger approximation introduced by a lower $\beta$ value. Note, however, that a solid explanation would be hard to provide in the absence of a deterministic global optimization algorithm, and the fact that local solvers can be impacted by how the problem settings change the sequence of iterations. It is interesting to note that in all the optimal scenarios obtained above (Figures 9, 12, and 15), the changeover path moves almost along the airline until it hits the boundaries of the flammability zone, where pure nitrogen starts to be added to the mixture. This is also evident from Figures 7, 10, and 13, where the inert inlet is almost zero until toward the end of the operation. For this reason, the fuel inlet valve is considered an additional decision variable here, unlike the purging operation where it was kept closed. The following final-time constraints are also enforced: the final methane composition $y_f(t_f) \geq y_{f_{min}} = 0.99$, and the final vessel pressure is to be within 7 and 8 bars. Two case studies are considered here. In the first one, the vessel is placed back into service after it has been purged previously using nitrogen (called warm filling). In the second one, the vessel is initially full of air under atmospheric conditions, for example, it is placed into service for the first time (called cold filling here). These cases are presented in the following subsections.

5.2. Safe Placing of Vessel into Service. The placing of a vessel into service is similar to the purging operation studied in Subsection 5.1 in that the same flammability zone must be avoided. However, the initial and final states of the vessel are different. In particular, the vessel starts from a mixture of air and nitrogen and is supposed to reach a state of almost pure fuel. For this reason, the fuel inlet valve is considered an additional decision variable here, unlike the purging operation where it was kept closed. The following final-time constraints are also enforced: the final methane composition $y_f(t_f) \geq y_{f_{min}} = 0.99$, and the final vessel pressure is to be within 7 and 8 bars. Two case studies are considered here. In the first one, the vessel is placed back into service after it has been purged previously using nitrogen (called warm filling). In the second one, the vessel is initially full of air under atmospheric conditions, for example, it is placed into service for the first time (called cold filling here). These cases are presented in the following subsections.

5.2.1. Warm Filling. Here, the vessel’s initial state is the final state of the previous purging operation. For example, the initial mole of (3.1, 20.2, and 291.1) for methane, oxygen, and nitrogen, respectively, as obtained in the previous subsection with $N = 6$ and $\beta = 2$ are considered (Figure 11). The 6 control intervals give rise to $6 \times 4 = 24$ optimization variables. As before, the smooth dynamic optimization is run with $\beta = 2$. The optimal valve openings and the corresponding inlet/outlet flow rates are given in Figure 16. The resulting optimal trajectories of the state variables and the optimal operation path are shown in Figures 17 and 18, respectively. For the warm filling scenario, the operation starts at $t = 0$ s from close to the bottom of the ternary diagram according to the initial mixture composition. Interestingly, the warm filling consumes no nitrogen as the inert content that is left in the vessel from the previous purge is enough for the filling operation to bypass the flammability zone. It should be noted that although the nitrogen valve is fully opened after $t = 50$ s, the inflow of nitrogen remains zero due to the negative pressure difference (note the check valves installed on the streams). In fact, there is a solution multiplicity in the optimal trajectory of
the nitrogen valve opening as both fully open and fully closed positions lead to zero flow, and in turn, an optimal value of zero for the nitrogen consumption (i.e., the objective function). It is also observed from Figure 17 that the final content of the vessel satisfies the problem constraints in terms of both methane mole fraction and vessel pressure.

The operation path (Figure 18) in the warm filling shows a direction change, where the methane mole fraction initially increases up to 35% around $t = 15$ s, and then, starts to go down until it reaches 20% at $t = 100$ s. This direction reversal can be explained from the flow rate and state trajectories in Figures 16 and 17, where it is seen that the flow of the incoming methane, which is supplied at 10 bar, keeps decreasing as the vessel pressure increases to and exceeds 10 bar (recall eqs 2 and 3 for pressure-flow relations). The methane flow finally stops as its corresponding valve is closed during $t \in [50, 100]$ s. At the same time, the air is entering at a higher flow rate, thereby decreasing the methane fraction in the vessel. An interesting point here is that the operation path illustrated in Figure 18 is not the only optimal solution yielding zero inert consumption. In fact, there are multiple optima in this case, one of which (found by manual trials) is given in Figures 19–21. This solution results in an operation path with no direction reversal while still keeping the inert consumption at zero.

5.2.2. Cold Filling. In this scenario, the vessel is considered to be initially full of air at the atmospheric pressure. Here again, $N = 6$ control intervals are used, leading to 24 optimization variables. This scenario turns out to be more challenging to solve than the warm filling. This is because according to Figure 1, the vessel is initially at point B, and there is no straight line from this point to point A without passing through the flammability zone. This means the optimizer must find appropriate trajectories of the valve openings that result in bypassing the flammability zone safely while also satisfying the other constraints in an optimal way.

As apparent from the thin non-flammable area around point B (Figure 1), the feasible region in cold filling is narrow. To help the optimizer converge successfully, a feasible set of initial...
guesses are chosen as follows. The nitrogen valve and the air valve are set to fully open and close, respectively, for the whole operation. The methane and outlet valves are set to fully open for the whole operation except the first interval where they are set to fully close. These initial guesses are obtained by manual trials and some engineering insights that initially no fuel or air should enter the vessel so that the operation remains in the narrow non-flammable region as it departs from point B (Figure 1). Although the foregoing initial guesses satisfy all the constraints of the original, nonsmooth problem, they happen to be infeasible for the smoothed problem with $\beta = 2$. In particular, they violate the flammability zone constraint. To show this graphically, the operation path obtained from the foregoing valve openings is shown in Figure 22, on which the approximate flammability zone after smoothing is also shown as a shaded area. It is seen that although the operation path is outside the nonsmooth flammability zone (i.e., the green dashed lines), it is clearly inside the smoothed flammability zone (i.e., the shaded area) at the beginning of the operation, rendering the initial guesses infeasible.

Figure 22 shows how smoothing can alter the actual feasible region by making it superficially larger or smaller. The alteration of the feasible region can negatively impact the optimization in two ways: (i) it can lead to sub-optimal results if parts of the feasible region containing a superior solution are excluded; (ii) it can lead to infeasibility (hence no convergence at all) if the feasible region becomes empty or too small that the local optimization algorithm fails to find a feasible solution (as observed in the present scenario). To mitigate the effect of smoothing on the feasible region, $\beta$ is increased to 25. The re-tuning of $\beta$ is supported by the fact that larger $\beta$ values result in less approximation errors, as shown in Figure 6.

The results of optimization with the abovementioned settings are illustrated in Figures 23–25. The narrow feasible path around the over-approximation of the flammability zone is particularly visible in Figure 25, where the operation starts at $t = 100$ seconds.

Figure 21. Optimal operation path corresponding to Figure 19, exhibiting no direction reversal.

Figure 22. Inflating effect of smoothing on the approximate nonsmooth flammability zone. The shaded area illustrates the approximate flammability zone after smoothing with $\beta = 2$.

Figure 23. Optimal valve openings and resulting flow rates for placing vessel into service using the smooth formulation with $N = 6$ and $\beta = 25$ (cold filling).

Figure 24. Optimal trajectories of state variables for placing vessel into service using the smooth formulation with $N = 6$ and $\beta = 25$ (cold filling).

Figure 25. Optimal operation path for placing vessel into service using the smooth formulation with $N = 6$ and $\beta = 25$ (cold filling).
0 from the bottom side of the diagram. It is also observed from Figures 23 and 25 how the operation is following a safe path by initially closing the fuel valve and pushing inert into the vessel. The optimal nitrogen used in this scenario is obtained as 668 mol.

To further see the effect of $\beta$ on the optimal results, it is increased to 60. As a result, the optimal nitrogen consumption is decreased to 572 mol in this case (i.e., about 15% more saving). The optimal trajectories are shown in Figures 26−28. The better solution with a larger $\beta$ can be attributed to the fact that approximation errors are reduced by increasing this parameter and the previous observation that lower $\beta$ values make for a smaller feasible region in this particular problem. Nonetheless, it is important to emphasize that whether a larger $\beta$ has a contracting, inflating, or mixed impact on the actual feasible region seems to be problem dependent. Such an impact would depend on the value of $\beta$ too, making it nearly impossible to reach a general verdict simply by manual trials. A general conclusion, if any, would require thorough mathematical analyses and simplifying assumptions, perhaps such as convexity, which are beyond the scope of this paper.

As the last experiment, the economic saving achieved by the optimization is investigated. For this purpose, the cold filling operation is performed with the most conservative procedure as follows: first, the vessel is emptied from air completely using nitrogen; then, the fuel is let in to push nitrogen out and yield a vessel full of fuel. No mixing of fuel and oxygen is allowed in this procedure. The trajectories for this procedure are shown in Figures 29−31. This operation requires 1595 mol of nitrogen, about three times higher than 572 mol, as obtained from optimization.

6. CONCLUSIONS AND FUTURE WORK

In this paper, the use of mathematical programming for optimal, safe operation of the changeover process is promoted. In particular, an optimization problem with a rather realistic dynamic model of the process is formulated. Although inert
minimization is considered as the objective in this work, other process objectives could also be used within the same formulation. The optimization problem features a safety constraint for avoiding the flammability zone, which is characterized by a new, simple nonsmooth formula that is able to over-approximate the flammability zone if additional margin of caution is desired. The non-differentiability of the underlying hybrid dynamic model and the new flammability zone characterization is circumvented by a direct smoothing strategy that uses adjustable sigmoid functions and avoids adding extra auxiliary variables or constraints as in previous work. The smoothing approach removes the need for complicated mixed-integer or complementarity reformulation of the nonsmoothness and keeps the problem small and easier to implement, maintain, and solve.

The following remarks are in order. The main objective of this work has been to show the benefits and practicality of dynamic optimization for safe changeover operations. Mathematical details have been presented to the extent necessary for motivating and understanding the work. Further theoretical analyses and numerical experimentation have been avoided and can be the subject of future research. For example, the implications of the smoothness parameter $\beta$ on the quality of the optimal solution have yet to be fully investigated. Such investigations would ideally need a deterministic global dynamic optimization algorithm. Otherwise, the effects of problem non-convexity and initial guesses preclude the possibility of general conclusions. It is, however, known that small $\beta$ values introduce larger approximations while offering better numerical properties than larger $\beta$ values, which reduce the approximation gap, while potentially causing issues with the numerical derivatives. Therefore, a trade-off is needed between good numerical properties and adequate fidelity to the original nonsmooth model. An adaptive (or optimization-based) procedure for finding the right $\beta$ can also be explored in the future. For the moment, an insight from similar approximation procedures suggests solving the problem repeatedly by starting with a small $\beta$ and increasing it each time, while using the optimal solution from the previous run as the initial guess for the current run. In this way, the optimal solution of the smooth problem would gradually approach that of the original nonsmooth problem.

From a practical perspective, uncertainties in the process model can affect the validity of the optimization results. To address uncertainties, which are important in safety applications, a robust extension of the proposed optimization problem can be pursued in the future. Also, the proposed framework can be applied to other practical safety problems such as systems with relief valves or safety interlocks that exhibit similar hybrid behavior. Moreover, the implementation of the proposed method in user-friendly software packages would help its adoption by process engineers and plant operators for economically safe changeover operations.

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