Optimal Start-Up of Air Separation Processes using Dynamic Optimization with Complementarity Constraints

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Abstract

Fluctuating electricity prices create an incentive for the flexible operation of electricity intensive processes, such as air separation units (ASUs). Shutting down an ASU during times with peak electricity prices has been claimed economically attractive but requires an efficient and largely automated start-up procedure. Previous works have considered simulations of plant start-ups and dynamic optimization of load scheduling near the nominal operation mode. Discrete events like the appearance of a liquid phase have impeded any rigorous ASU start-up optimization. In this work, we formulate the optimal start-ups as dynamic optimization problems with regularized algebraic complementarity constraints (Caspari et al., 2019b) using a mechanistic dynamic process model in Modelica. Our approach captures physical effects appearing during start-up like the appearance and disappearance of phases. We solve the resulting optimization problems with direct single-shooting using the dynamic optimization framework DyOS. We perform in-silico dynamic offline optimizations of an ASU start-up and consider different process modifications. We consider cold start-up optimizations, where the process medium is initialized at cryogenic conditions just before liquefaction. The results illustrate that the proposed approach can be applied to large-scale processes. The results show further that liquid assist operation reduced the optimal start-up time by about 70\% compared to the start-up without this modification.

Keywords: dynamic optimization, complementarity constraints, air separation, optimal start-up

1. Introduction

The flexible operation of continuous processes in the presence of fluctuating electricity prices enable economic benefits (Daryanian et al., 1989). Since air separation units (ASUs) are large-scale electricity consumers, they are well suited for exploiting electricity price fluctuations (Caspari et al., 2019c). Irrespective of the different
perspectives on flexible operation, whether scheduling (Zhang et al., 2015) or control (Huang et al., 2009), the start-up or shut-down of processes have been either assumed to be known or neglected; estimates of the start-up or shut-down times are used in the transitional constraints in scheduling and the control approaches assume the process to be in operation around nominal conditions. However, start-up and shut-down are crucial for the exploitation of the economic potential when the electricity price dynamics and process dynamics are in the same range, like in the case of ASUs (Miller et al., 2008b). While start-ups are currently performed with a fixed recipe under the surveillance of skilled workers, a rigorous optimization-based approach would be desirable leading to faster commissioning, higher energy efficiency, and reduced labour (Vinson, 2006). While simulations of an ASU start-up has been reported in literature, e.g., (Kender et al., 2019; Miller et al., 2008a), the optimization of a start-up process has not yet been considered. The optimization has to deal with discrete events like the appearance and disappearance of phases. The ASU can be described by a nonsmooth differential algebraic equation (DAE) system and the start-up optimization can be formulated as a dynamic optimization problem with complementarity constraints (CCs). Optimization problems of this form have been solved using full discretization leading to a nonlinear program (NLP) with equilibrium constraints, e.g., (Raghunathan et al., 2004). Recently, we proposed an approach for the efficient solution of such problems based on direct shooting (Caspari et al., 2019b). In this work, we apply this approach for the start-up optimization of an ASU. The start-up optimizations allow us to evaluate different process designs regarding their impact on the start-up. We therefore consider liquid assist operation in addition to a basic process design and perform start-up optimizations for both designs. We consider a cold process start-up, i.e., we assume the medium in the process to be already at cryogenic conditions, just before liquefaction. A warm start-up would assume that the medium inside the process is at ambient conditions. The cold start-up occurs when the plant was shut down for no more than several hours up to a few days (Miller et al., 2008a), which covers most of the scenarios occurring during flexible operation of an ASU. This could be the case in an operation scenario where the process is turned-off in the presence of very high electricity prices and turned-on otherwise. We briefly describe the process and its model in Section 2 and summarize the problem formulation and solution approach in Section 3. We show the results in Section 4 and conclude in Section 5.

2. Process and Model

We consider the ASU depicted in Figure 1, which is similar to the process we used in (Caspari et al., 2018). Ambient air (nitrogen, oxygen, argon) enters the process, is
compressed to 11 bar, inter-cooled to 298 K and fed to the heat exchanger. There, the air stream is cooled in counter current with the waste and the gaseous nitrogen product (GNP) stream. A part is split-up and expanded to the column feed pressure in a turbine. The remaining part enters zone 2 of the heat exchanger, where it is further cooled and may be liquefied. Both streams are mixed and fed to the column. The condenser pressure is 5.5 bar whereas the reboiler outlet pressure is 1.5 bar. We adapt the liquid assist modification proposed in Miller et al. (2008a) for an ASU with an argon column; the GNP stream is liquefied and stored in a tank and can be fed into the column top stage to accelerate the process start-up. We implement a mechanistic dynamic model that is able to represent the transient process behaviour during the ASU start-up. The model includes CCs for modelling the appearance and disappearance of vapour-liquid equilibria (VLEs), overflow weirs and valves. It uses a relaxed VLE formulation similar to (Raghunathan et al., 2004), which includes CCs of the form $0 \leq y_{ik}(t) \perp y'_{ik}(t) \geq 0$. We apply similar formulations with CCs for overflow weirs and vapor outlet streams valves of the column trays. We briefly summarize the model and refer to previous works. We use the unit models from (Caspari et al., 2019b), the column model and the relaxed VLE formulation from (Raghunathan et al., 2004), and the physical property models from Johansson (2015). Thermodynamics: The vapour phase is modelled as an ideal gas and the liquid phase as a nonideal liquid. We apply standard models for the physical properties. We refer to Johansson (2015). Distillation Column: We use the same distillation column model as in (Raghunathan et al., 2004) with 40 trays. The model includes vapour and liquid holdsups. Every tray has an overflow weir. The vapour outlet is calculated based on the pressure difference between the trays. Every tray includes 4 CCs: for the liquid outlet, the gas outlet, and two for the relaxed VLE. Consequently, the column model includes 160 CCs. PHX: We use a 1-dimensional distributed model for the heat exchangers. The fluid behaves quasistationary. We consider dynamic energy balances for the wall. Liquefaction can take only place in the PHX2 in the feed air stream, justified by several simulations. The PHX1 has 50 finite elements. We use 1 finite element for the PHX2. The PHX 2 include 2 CCs for the VLE. Compressor/Turbine: The compressor and turbine are modelled with an adiabatic efficiency of 0.8. The turbine includes 2 CCs for the relaxed VLE. Integrated reboiler and condenser: We model the reboiler as an equilibrium tray with a heat supply and the condenser as pseudo-steady-state. Reboiler and condenser are energetically integrated using a heat transfer correlation. The reboiler includes 4 CCs. The condenser includes 2 CCs for the VLE. Liquefier: We model the liquefier with a liquefaction efficiency of 0.8. The resulting process model is a differential index 1 DAE including 270 differential and about 3060 algebraic states. The model includes 170 CCs.

3. Problem Formulation and Solution Approach

The optimal start-up problems are formulated as a dynamic optimization problem with algebraic CCs. We described how to handle these in single shooting in detail in our previous work (Caspari et al., 2019b): We substitute each CCs using a regularized Fischer-Burmeister function of the form $0 = y_{ik}(t) + y'_{ik}(t) - \sqrt{y_{ik}(t)^2 + y'_{ik}(t)^2 + \varepsilon, \varepsilon > 0}$. The Fischer-Burmeister function is directly used as model equation. Regularization of the Fischer-Burmeister function leads to a smooth DAE, enabling the application of standard integrators and optimizers to solve the optimization problems using direct shooting. We minimize the deviation of the GNP purity $x_{GNP}$, the GNP flowrate $n_{GNP}$, the liquefier splitfactor $\xi_{liq}$ and the tank holdup $n_{tank}$ from there desired setpoints by using the following objective function: $\Phi =$
\[ \int_0^T \left( w_{\text{pur}} (x_{\text{GNP}}(t) - x_{\text{GNP}}^{\text{set}})^2 + w_{\text{flow}} (n_{\dot{\text{GNP}}}(t) - n_{\text{GNP}}^{\text{set}})^2 + w_{\text{liq}} (\xi_{\text{liq}}(t))^2 \right) \, dt, \]

with the weight parameters

\[ w_{\text{pur}} = 10^{-3}, \quad w_{\text{flow}} = 10^{-3}, \quad w_{\text{liq}} = 10^{-4}, \quad w_{\text{tank}} = 10^{-10}, \quad x_{\text{GNP}}^{\text{set}} = 0.99995, \quad n_{\text{GNP}}^{\text{set}} = 150 \text{ mol/s}. \]

We penalize the liquefier stream, since the liquefication uses electricity and could thus be used as a bonus reflux for the column; we aim to minimize the liquefier activity in order to keep the electricity demand as low as possible while still allowing its use for the tank refill. We penalize the deviation of the tank holdup from the initial value to avoid unnecessary tank withdrawal. We use the following controls and bounds:

\[ \xi_{\text{PHX}}(t) \in [0.85, 0.95], \quad \xi_{\text{LP}}(t) \in [0.2, 0.8], \quad \xi_{\text{liq}}(t) \in [0.5, 1], \quad n_{\dot{\text{air}}}(t) \in [300, 340] \text{ mol/s}, \quad n_{\text{assist}}(t) \in [0, 30] \text{ mol/s}. \]

The control variables are initialized with the constant profiles

\[ \xi_{\text{PHX}}(t) = 0.9, \quad \xi_{\text{LP}} = 0.5, \quad \xi_{\text{liq}} = 1, \quad n_{\dot{\text{air}}} = 320 \text{ mol/s}, \quad n_{\text{assist}} = 0 \]

and are discretized piecewise constant with 60 intervals. We use the path constraints

\[ \phi_{\text{turbine}}(t) \in [0.85, 0.95], \quad x_{\text{tank}}(t) \in [0.99995, 1]. \]

The turbine vapour fraction is constrained due to technical limitations of the turbine. The tank purity is constrained to the nominal product purity to avoid contamination in the tank. The last two summands of the objective function with the respective weights, the liquefier split factor, and the liquid assist flowrate are used only in the case with liquid assist operation. We assumed the start-up procedure to be finished when the product purity and the product flowrate are at their desired setpoints. We implement the process model in Modelica and use direct single-shooting (Brusch and Schapelle, 1973) to solve the optimization problems with the shooting framework DyOS (Caspari et al., 2019a). The DAE integrator is NIXE (Hannemann et al., 2010) and the NLP solver is SNOPT (Gill et al., 2005). We use integration tolerances of \(10^{-6}\), NLP tolerances of \(10^{-4}\).

4. Numerical Results

4.1. Start-Up without Liquid Assist Operation

Figure 2 shows results from the dynamic optimization of the start-up without liquid assist operation. The start-up time is about 1.5 h (Figures 2d and 2e). At the beginning, the turbine activity is at the maximum (Figure 2a), while the air feed flowrate is at the lower bound (Figure 2b), and the column split factor is increased (Figure 2c) leading to a higher column reflux. This supports the cooling of the medium in the process since the turbine withdraws energy from the process and the reduced feed air flowrate reduces the energy fed to the process through the air feed. We see that the amount of liquid in the column increases.

Figure 2: Optimal control and state variable profiles for start-up without liquid assist operation.

Start-up range indicated by vertical, dotted lines. (a) PHC split factor to turbine. (b) Feed air flowrate. (c) Column split factor. (d) GNP flow rate. (e) GNP purity. (f) Column tray holdups.
starting with the first tray followed by the other trays (Figure 2f). With the optimal control profiles, the product flowrate increases in the beginning before it settles down to the setpoint (Figure 2d). The product purity begins from ambient conditions and increases until it reaches the desired setpoint (Figure 2e).

4.2. Start-Up with Liquid Assist Operation

Figure 3 shows results from the dynamic optimization of the start-up with liquid assist operation. The optimal start-up takes about 24 min (Figures 3d and 3e), which corresponds to a reduction of the optimal start-up time of about 70% compared to the optimal startup without liquid assist operation. The control variable profiles for the PHC splitfactor (Figure 3a), the feed air flowrate (Figure 3b), and the column splitfactor (Figure 3c) look qualitatively similar to the case without liquid assist operation (Figure 3c). The start-up is clearly supported by the liquid assist operation: The assist stream is at the upper bound in the beginning before it is reduced and set to zero at the end (Figure 3f). Remember that we penalize the liquid assist flowrate. The liquefier is used to refill the tank, in which the holdup is decreased due to the liquid assist stream. The tank refill is induced by the holdup penalization. However, due to the tank purity constraint, the liquefier can only be activated if the GNP purity is suitable and does not pollute the tank. The liquefier is thus activated as soon as the GNP purity is at the desired value (Figures 3g and 3e). The state variable profiles, e.g., for the product flowrate and purity (Figures 3d and 3e) look qualitatively similar as for the case without liquid assist option, though the operating level is obtained faster.

5. Conclusions

We use dynamic optimization with CCs to optimize start-ups of an ASU. The optimizations allow to evaluate process design modifications with respect to the effect on the process start-up time. We therefore perform cold start-up optimizations for ASU designs with and without liquid assist option. The results demonstrate the applicability of the approach to large-scale processes. They show further the effectiveness of liquid assist operation. This modification reduces the optimal process start-up time by about 70% compared to a start-up without this modification. Further work can consider the start-up of ASUs with additional design modifications, other topologies, a warm process start-up starting from ambient conditions, and the application of the obtained start-up procedure.
to a real process. Future work can use the approach to obtain start-up and shut-down times as required for transitional constraints in scheduling, and for online control.

**Acknowledgement:** The authors gratefully acknowledge the financial support of the Kopernikus project SynErgie by the Federal Ministry of Education and Research (BMBF) and the project supervision by the project management organization Projektträger Jülich (PtJ). The authors thank Anna-Maria Ecker, Florian Schliebitz, Gerhard Zapp from the Linde AG for fruitful discussion.

**References**


